

## **Phase Transformations in Pressure Polymerized C60: Enthalpies and Kinetic Parameters**

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Differential Scanning Calorimetry (DSC) and IR- spectroscopy were used to monitor the depolymerization of the three pressure polymerized phases of C60 : rhomboheral (R); orthorhombic (O) and tetragonal (T) into C60 fcc. The mechanism of decomposition of the three phases is significantly different, which is clear even from the shapes of the DSC peaks. R to C60 fcc transformation is at least a two-step process, as proved by IR-monitoring. It includes decomposition of R into short fragments (dimers, trimers, non-linear plain structures) first and later the formation of C60 fcc. No IR-detectable intermediate species were found while decomposition of O and T phases. The transformation enthalpies of R-, O-, T- into C60 fcc were measured. The R / fcc C60, O / fcc C60 and R / O phase boundaries were sketched in. The equilibrium phase diagram obtained was compared with the "phase map", which shows pressure and temperature conditions of a preparation of each phase.

Degree of conversion ( $\alpha$ ) vs. time (t) vs. temperature (T) dependencies were obtained for the decomposition of O - phase into C60 fcc using IR, DSC or combination of both. The one - step process was described with the effective pre-exponential factor  $\ln k = 35 \pm 5$ , activation energy  $E = 170 \pm 20$  kJ/mol and the order of a reaction,  $n = 0.8$ .