Effects of hard- and soft-segment composition on pyrolysis characteristics of MDI, BD, and PTMG-based polyurethane elastomers

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Abstract:
A study of the morphology changes in polyurethane elastomers (PUEs) containing different hard- and soft-segment ratios during ramped-heating pyrolysis revealed that selectivity of urethane bond cleavage is controlled by only the segment composition. Several PUEs were synthesized using 4,4’-diphenylmethane diisocyanate, 1,4-butanediol, and poly(oxytetramethylene glycol) (PTMG) to examine the influence of segment composition on pyrolysis characteristics by pyrolysis–gas chromatography/mass spectrometry, evolved gas analysis–mass spectrometry, and isoconversional kinetic studies. Soft-segment-rich PUEs tended to undergo urethane bond cleavage via a 4-membered-ring transition state, while the linkages in other compositions were selectively cleaved via a 6-membered-ring transition state. The reaction selectivity can be explained by the different conformations of the urethane bonds: in the hard-segment domains by H-bonds between urethane unit NH and CO groups, and in soft-segment-rich environments by H-bonds between urethane NH groups and PTMG O linkages. The mechanism of PTMG pyrolysis was the same for all PUEs.

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Frontier Labs Products used:
Multi-Shot Pyrolyzer (EGA/PY-3030D), UA*-1, UA-DTM-2.5N