AN XRD, FT-IR AND COMPUTATIONAL ANALYSIS OF NANOSTRUCTURE OF SINGLE AND MIXED γ-ALUMINA AND THORIUM OXIDE

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Mixed γ-alumina and thorium oxide were prepared with various compositions (between 100, 95, 90, 80, 50, 25, 15, 5 and 0 wt%, respectively) by addition of solution of thorium nitrate to a slurry solution of aluminum isopropoxide [$Al(OC_3H_7)_3$] in deionized water. Mixed oxides (slurry solution) were heated at 120 ^oC (oil bath) for 24h with mixing (for uniform distribution of oxides and to remove excess water) followed by calcinations at 600 ^oC for 6h. New FT-IR absorption bands and absence of crystallinity demonstrated by XRD analysis clearly show that γ-alumina and thorium oxide are mixed chemically and on atomic scale during the calcination period. The mechanically mixed oxide retained crystallinity and does not show mixing on atomic scale. The evaluation for the catalytic activity of single or the chemically mixed catalysts for the dehydration of 2-hexanol and 1,2-diphenyl-2-propanol was investigated. Computational analysis of nanostrcture of γ-alumina (calculated by AM1 method) show absorption pattern similar to FT-IR.