

Metastable dimethyl phthalate molecular ions: Does the loss of a methoxyl radical proceed with or without anchimeric assistance?

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Abstract: Using MS/MS/MS experiments and quantum chemical calculations, it is demonstrated that oxygen (carbonyl) methylated phthalic anhydride cations are produced when metastable dimethyl phthalate molecular ions expel a methoxyl radical. At higher internal energies, isomeric acyl ions are competitively generated. © 2009 Elsevier B.V. All rights reserved.

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