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Modeling chemical reactions in classical molecular dynamics simulations

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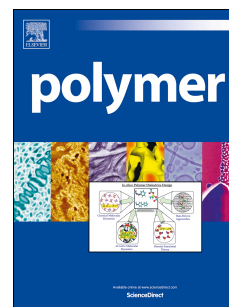
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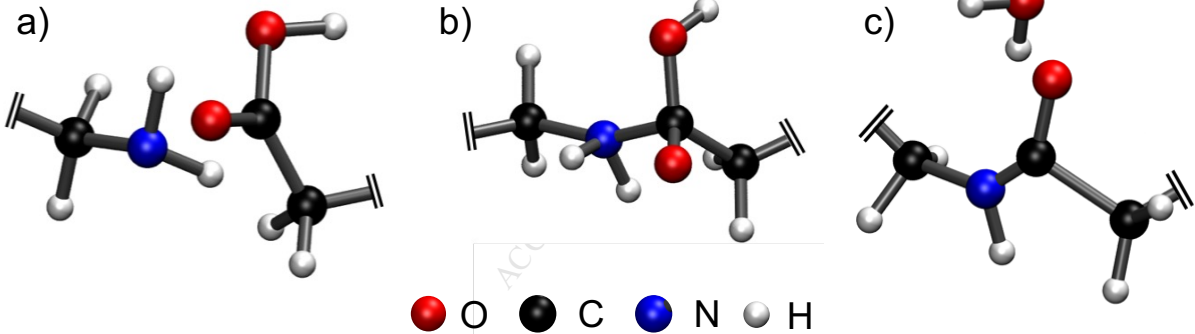
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