

Abbreviations

a.u.	atomic units
B3LYP	Becke, 3-parameter, Lee-Yang-Parr hybrid functional
BCP	bonding critical point
CH₃CH₃	NC repeat unit with two methoxy capping groups
CH₃OH	NC repeat unit with a methoxy capping group on ring 1, hydroxy capping on ring 2
CCP	cage critical point
CP	critical point
DFT	density functional theory
DOS	degree of substitution
EM	energetic materials
ESP	electrostatic potential
G09	Gaussian 09 revision D.01
GM	genetically modified
GView	Gauss View 5.0.8
HF	Hartree Fock theory
IR	infra-red spectroscopy
MEP	minimum energy path

MM	molecular mechanics
MMFF94	Merck molecular force field 94
MW	molecular weight
NC	nitrocellulose
NCP	nuclear critical point
NG	nitroglycerine
NMR	nuclear magnetic resonance spectroscopy
OHCH₃	NC repeat unit with hydroxy capping group on ring 1, methoxy capping group on ring 2
PES	potential energy surface
PETN	pentaerythritol tetranitrate
QM	quantum mechanics
QTAIM	quantum theory of atoms in molecules
RCP	ring critical point
SEM	scanning electron microscopy
S_N2	bi-molecular nucleophilic substitution reaction
TS	transition state
UFF	universal force field
ωB97X-D	ω B97X-D long-range corrected hybrid functional

Chapter 1

Post-Denitration Reactions

1.1 Introduction

Following denitration, the products can be evolved as gases or remain in the nitrocellulose (NC) matrix.

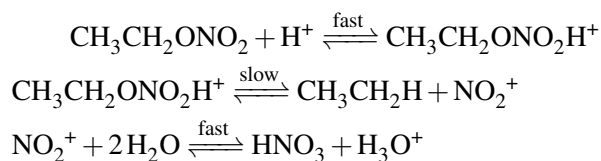
1.2 Computational details

1.3 Thermodynamics of Ethyl Nitrate reactions

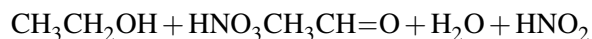
For an in ital comparison of the methods you used, you could do a diagram like the one Kukulja did (kukulja2014.pdf, page 89, fig 3.7). She also makes mention of the overestimation of activation barriers for pure DFT methods. Make sure you know the background surrounding this - why does this occur, and what is done to remedy it?

Camera' equations

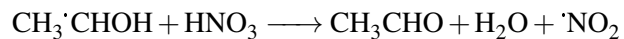
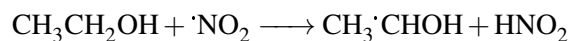
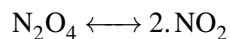
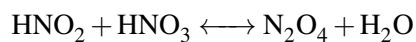
Hydrolysis



Initiation

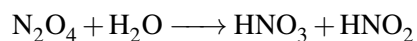
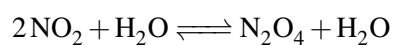


Propagation

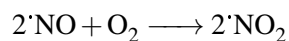
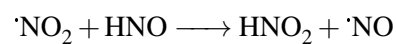
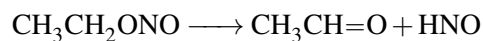
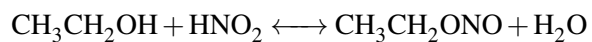


Aellig's equations

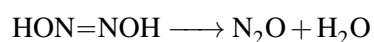
Initiation



Propagation



Termination



1.3.1 Radical mechanistic route

1.3.2 Ionic mechanistic route

1.4 Reactions of Nitrocellulose Monomer

1.5 Summary