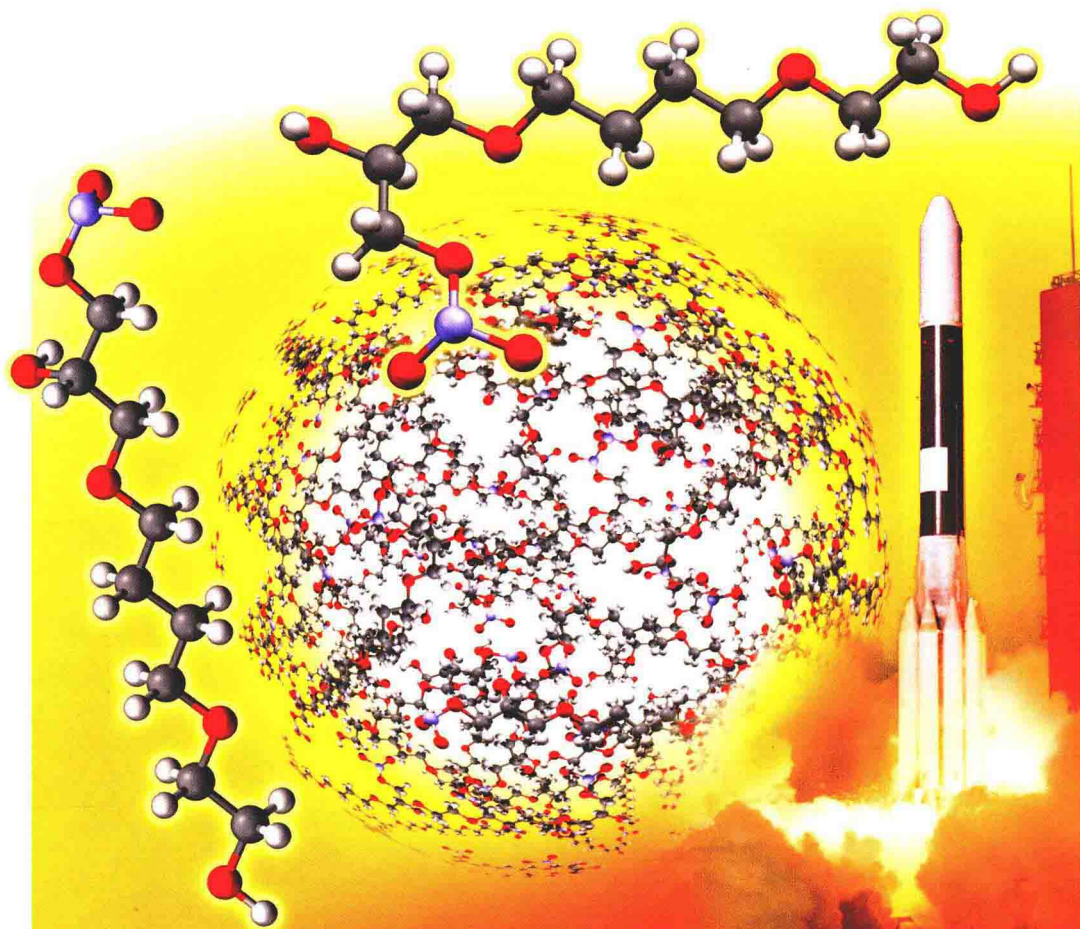


How Ghee Ang and
Sreekumar Pisharath

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Energetic Polymers

Binders and Plasticizers for Enhancing Performance



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Preface

Over the years, a variety of polymer binders have been developed and used in energetic material composite applications to cope with the global demand for insensitive and high performance propellant and explosive formulations. One of the important milestones in this effort was the development of polymers containing energetic groups, namely azido or nitro groups that release significant amounts of energy under the application of a thermal stimulus. Such type of polymers are referred as energetic polymers. Energetic polymers, when used as binders, provide additional energy and insensitivity to formulations as compared with their inert counterparts. Low molecular weight energetic polymers, with the advantages of a lower migration tendency and less sensitivity to external stimuli, are finding application as energetic plasticizers. Through the years, a range of energetic polymers have been developed as prospective candidates for application as binders and plasticizers. Some of them, namely GAP, Poly(NIMMO), and Poly (GLYN), have reached the stages of mass production.

This book is intended to provide a state-of-the-art overview of the various energetic polymers employed for propellant and explosive formulations. The book is divided into seven chapters. The first chapter details the historical development of the emergence of polymers, including that of the energetic ones, as a vital component in energetic material composites. Chapters 2 and 3 discuss the two important members of the energetic polymer family; the high nitrogen containing polymers and nitropolymers. For the former, the high nitrogen content (in the form of azido and tetrazole groups) provides the polymers with high positive heat of formation and superior energetic properties, albeit resulting in fuel-rich formulations. However, for the latter, the presence of nitro groups offers a better balance of oxygen content and energetic properties. The majority of the commercialized energetic polymers for binder and plasticizer applications belong to these two families. Comparisons are provided wherever possible with the inert binder formulations, to stress the capability of energetic binder formulations for enhancing performance and insensitivity.

Energetic thermoplastic elastomers (ETPEs) have evinced an immense interest due to their unique mechanical and thermal behavior. They are copolymers of energetic polymers that are discussed in Chapters 2 and 3. ETPEs provided a paradigm shift in the processing of energetic material formulations by replacing

the cast curing process with an environment friendly melt casting process. Chapter 4 presents the various ETPEs used as binders and their application in propellant and explosive formulations.

The application of fluoropolymers as binders is discussed in Chapter 5. Fluoropolymers owe their reactivity to the high electronegativity and oxidizing nature of fluorine. Higher combustion energies could be obtained from composites of fluoropolymers with nanoparticles of combusting metal fuels, such as magnesium and aluminum. This possibility has opened up a new area of energetic materials research called reactive nanomaterials.

Plasticizers derived from energetic polymers with nitro and azido substituents have lower migration tendency as compared with the nitrate ester based energetic plasticizers used in explosive and propellant formulations. The preparation, physical properties, and energetics of azido/nitro polymer based energetic plasticizers are discussed in Chapter 6.

The macroscopic behavior of energetic material composites is the result of the complicated physical processes and microstructure occurring in the composite at multiple length and time scales. Therefore, a multiscale simulation approach is necessary for the prediction of macroscopic properties of energetic material composites from fundamental molecular processes. Simulation of such systems requires theoretical models that range from those including atomistic effects to macroscopic continuum models and passing through the intermediate mesoscopic simulations. Chapter 7 introduces the concept of multiscale modeling in energetic composites and application to simulate the physical and chemical processes in the energetic composites. We hope that the energetic polymers and formulations presented here will be useful in enhancing the search for new high performance and insensitive energetic material composites.

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Abbreviations

| | |
|---------|--|
| A | Frequency Factor |
| AA | Acrylic acid |
| ABL | Allegheny Ballistics Laboratory |
| AC | Acrolyl chloride |
| ACE | Activated Chain End |
| ADN | Ammonium dinitramide |
| ADDF | 2,2-Dinitro-1,3-propanediol diformate |
| AFM | Atomic Force Microscopy |
| AFEM | Atomic-Scale Finite-Element Method |
| AIAA | American Institute of Aeronautics and Astronautics |
| AMM | Activated Monomer Mechanism |
| AMMO | 3-Azidomethyl 3-methyl oxetane |
| AN | Ammonium nitrate |
| AP | Ammonium perchlorate |
| ARC | Adiabatic Reaction Calorimetry |
| ARL | Army Research Laboratory, USA |
| ASME | American Society of Mechanical Engineers |
| AWE | Atomic Weapons Establishment, UK |
| BABAMP | Bis(azido acetoxy) bis(azido methyl) propane |
| BAMO | 3,3-Bis(azidomethyl) oxetane |
| BBrMO | 3,3-Bis(bromomethyl) oxetane |
| BCMO | 3,3-Bis(chloromethyl) oxetane |
| BDO | 1,4-Butanediol |
| BDNPA | Bis(2,2-dinitropropyl) acetal |
| BDNPF | Bis(2,2-dinitropropyl) formal |
| BDNPA/F | Bis(2,2-dinitropropyl) acetal/formal |
| BE | Boundary Element |
| BTTN | 1,2,4-Butanetriol trinitrate |
| BTATz | 3,6-Bis(1H-1,2,3,4-tetrazol-5-ylamino)-s-tetrazine |
| Bu-NENA | Butyl-N-(2-nitratoethylnitramine |
| B3LYP | Becke 3-Parameter (Exchange) Lee Yang Parr |
| CAB | Cellulose acetate butyrate |
| CAL | Calorie |

| | |
|---------------|--|
| CC | Copper chromite |
| CD | Cyclodextrin |
| CDN | Nitrated cyclodextrin |
| CEP | Tris(β -chloroethyl) phosphate |
| CFC | Chlorofluorocarbon |
| CG | Coarse Grain |
| CL-20 | 2,4,6,8,10,12-Hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane (HNIW) |
| CLMMO | 3-Chloromethyl-3-methyl oxetane |
| CMDB | Composite Modified Double Base |
| Comp. B | Explosive composition based on RDX and TNT |
| COMPASS | Condensed-phase Optimized Molecular Potentials for Atomistic Simulation Studies |
| CPX-413 | UK's extremely insensitive explosive composition based on NTO, HMX, and Poly(NIMMO). |
| CRP | Controlled Radical Polymerization |
| CTPB | Carboxy terminated polybutadiene |
| CTFE | Chlorotrifluoroethylene |
| DAAF | 4,4-Diamino-3,3-azoxyfurazan |
| DB | Double Base |
| DBTDL | Dibutyltin dilaurate |
| DBP | Dibutyl phthalate |
| <i>p</i> -DCC | <i>p</i> -Bis (α,α -dimethylchloromethyl) benzene |
| DDM | 4,4'-Diaminodiphenylmethane |
| DEGBAA | Diethylene glycol bis-azido acetate |
| DEGDN | Diethylene glycol dinitrate |
| DHT | 3,6-Dihydrazino-s-tetrazine |
| DMA | Dynamic Mechanical Analysis |
| DMSO | Dimethyl sulfoxide |
| DMF | Dimethyl formamide |
| DNAN | 2,4-Dinitroanisole |
| DPD | Dissipative Particle Dynamics |
| DOS | Diocetyl sebacate |
| DREV | Defense Research Establishment Valcartier, Canada |
| DSC | Differential Scanning Calorimetry |
| DSTO | Defence Science and Technology Organization |
| DTA | Differential Thermal Analysis |
| DTG | Derivative Thermogravimetric Analysis |
| DTIC | Defense Technical Information Center |
| DRA | Defense Research Agency, UK |
| E_A | Activation energy |
| ECH | Epichlorohydrin |
| EGBAA | Ethylene glycol bis-azido acetate |
| EGDN | Ethylene glycol dinitrate |
| EIDS | Extremely Insensitive Detonating Substance |

| | |
|---------------------|--|
| EOS | Equation of State |
| ETPE | Energetic Thermoplastic Elastomer |
| Et-NENA | Ethyl- <i>N</i> -nitrateoethylnitramine |
| ESD | Electrostatic Discharge |
| ESA | European Space Agency |
| ESR | Electron Spin Resonance |
| ESTANE | Thermoplastic elastomer based on segmented polyurethane |
| FOI | Swedish Defence Research Agency |
| F of I | Figure of Insensitivity |
| FOX-7 | 1,1-Diamino-2,2-dinitroethylene |
| FK-800 | A fluorocopolymer developed by 3M having equivalent composition to that of Kel-F800 |
| FTIR | Fourier Transform Infrared |
| GA | Glycidyl azide |
| GAP | Glycidyl azide polymer |
| GAPA | Azido terminated GAP |
| GC | Gas Chromatography |
| GLyN (GN) | Glycidyl nitrate |
| GPC | Gel Permeation Chromatograph |
| GZT | Guanidine-5,5'-azotetrazolate |
| H-6 | Underwater explosive composition developed by Australia |
| HDPE | High Density Polyethylene |
| HFP | Hexafluoropropylene |
| HFC | Heat Flow Calorimetry |
| HMMO | 3-Hydroxy methyl-3-methyl oxetane |
| H ₁₂ MDI | 4,4'-Dicyclohexyl methyl diisocyanate (4,4'-diphenylmethane diisocyanate) |
| HMX | High Melting Explosive or Her Majesty's Explosive |
| HNF | Hydrazinium nitroformate |
| HOMO | Highest Occupied Molecular Orbital |
| HTPB | Hydroxy Terminated Polybutadiene |
| HYFLON | Fully fluorinated semicrystalline copolymer of tetrafluoroethylene (TFE) and 2,2,4-trifluoro-5-trifluoro-methoxy-1,3-dioxide (TTD) |
| ICE | Isentropic Compression Experiment |
| ICI | Imperial Chemical Industries |
| ICT | Fraunhofer Institut Chemische Technologie, Germany |
| IM | Insensitive Munition |
| IMEMTS | Insensitive Munitions and Energetic Materials Technical Symposium |
| IPDI | Isophorone diisocyanate |
| I_{sp} | Specific Impulse |
| IDP | Isodecyl pelargonate |
| J | Joule |
| JANNAF | Joint Army–Navy–NASA–Air Force |
| JA2 | Nitrocellulose based propellant |

| | |
|----------|---|
| JAX | JA2 propellant loaded with RDX |
| K | Kelvin |
| K-10 | A mixture of 2-nitroethylbenzene and 2,4,6-trinitroethylbenzene |
| Kel-F800 | Copolymer of vinylidene and hexafluoropropylene |
| Kraton | Copolymer of styrene and ethylene/butylenes |
| LANL | Los Alamos National Laboratory |
| LLNL | Lawrence Livermore National Laboratory |
| LLM-105 | 2,6-Diamino-3,5-dinitropyrazine-1-oxide |
| LOVA | Low Vulnerability Ammunition |
| LUMO | Lowest Unoccupied Molecular Orbital |
| LX | Series of explosive formulations developed by LLNL based on fluoropolymer binders |
| MAPO | Tris(1-(2-methylaziridinyl) phosphine oxide) |
| MCHI | Methylene bis(cyclohexyl isocyanate) |
| MD | Molecular Dynamics |
| MHMO | 3-Methyl 3-hydroxymethyl oxetane |
| MIL-STD | Military Standard |
| MMA | Methyl methacrylate |
| M_c | Average molecular weight between crosslinks |
| M_n | Number average molecular weight |
| M_w | Weight average molecular weight |
| Me-NENA | Methyl- <i>N</i> -(2-nitroxyethyl) nitramine |
| MODPOT | <i>Ab initio</i> Core Model Potential |
| MOVO | Molybdenum/vanadium oxide catalysts |
| MRD-CI | Multiple Reference Double Excitation–Configuration Interaction |
| MS | Mass Spectroscopy |
| MSIAC | Munitions Safety Information Analysis Center |
| MTH | Mathematical Theory of Homogenization |
| MTMO | 3-Methyl-3'-(tosyloxymethyl) oxetane |
| NASA | National Aeronautic Space Agency |
| NATO | North Atlantic Treaty Organization |
| NC | Nitrocellulose |
| NCO | Isocyanate |
| NDIA | National Defence Industrial Association |
| NENA | <i>N</i> -(2-nitroxyethyl) nitramine (nitrateethylnitramine) |
| NG | Nitroglycerin |
| NHTPB | Nitrated hydroxy terminated polybutadiene |
| NIMMO | 3-Nitratomethyl 3-methyl oxetane |
| NIMIC | NATO Insensitive Munitions Information Center, USA |
| NMR | Nuclear Magnetic Resonance |
| NSWC | Naval Surface Warfare Centre |
| NTO | 3-Nitro-1,2,4-triazole-5-one |
| OB | Oxygen Balance |
| ODTX | One Dimensional Time to Explosion |
| OM | Optical Microscopy |

| | |
|----------------------|---|
| ONR | Office of Naval Research |
| P1 | 1,3-Bis{azidoacetoxy}-2-azidoacetoxymethyl-2-ethylpropane |
| PEAA | 1,3-Bis{azidoacetoxy}-2,2-bis{azidomethyl} propane |
| PAN | Polyacrylonitrile |
| PAX | Picatinny Arsenal Explosive |
| PB | Polybutadiene |
| PBA | Poly(butylene adipate) |
| PBAA | Poly(butadiene–acrylic acid) |
| PBAN | Poly(butadiene–acrylic acid–acrylonitrile) |
| PBX | Polymer Bonded Explosive |
| PBXW-115 | PBX developed in USA for underwater applications |
| PBXN | PBXs developed by US Navy |
| P_{CJ} | Chapman–Jouguet Pressure |
| PCTFE | Polychlorotrifluoroethylene |
| PDMS | Poly(dimethyl siloxane) |
| PECH | Poly(epichlorohydrin) |
| PEG | Polyethylene glycol |
| PETKAA | Pentaerythritol tetrakis (azidoacetate) |
| PMMA | Poly(methyl methacrylate) |
| PMVT | Poly(2-methyl-5-vinyl tetrazole) |
| PNC | Polymer Nanocomposite |
| Poly(AMMO) | Poly(3-azidomethyl 3-methyloxetane) |
| Poly(BAMO) | Poly(3,3-bis(azidomethyl) oxetane) |
| Poly(BEMO) | Poly(bis(ethoxymethyl) oxetane) |
| Poly(CDN) | Nitrated cyclodextrin polymers |
| Poly(GlyN) or PGN | Poly(glycidyl nitrate) |
| Poly(NiMMO) | Poly(3-nitratomethyl 3-methyl oxetane) |
| Pr-NENA | Propyl- <i>N</i> -(2-nitroxyethyl) nitramine |
| Pe-NENA | Pentyl- <i>N</i> -(2-nitroxyethyl) nitramine |
| PS | Poly(styrene) |
| PTC | Phase Transfer Catalyst |
| PTFE | Poly(tetrafluoroethylene) |
| PU | Polyurethane |
| PVT | Poly(vinyl tetrazole) |
| PVDF | Poly(vinylidene difluoride) |
| QM | Quantum Mechanics |
| QRX077 | Explosive formulation containing HMX, FOX-7, and inert binder |
| RDX | Research Department Explosive |
| RVE | Representative Volume Element |
| SBAT | Simulated Bulk Auto-Ignition Temperature |
| SEM | Scanning Electron Micrograph |
| SMATCH | Simultaneous Mass and Temperature Change |
| SNPE | Societe Nationale des Poudres et Explosifs, France |
| T | Absolute Temperature |

| | |
|-------|--|
| T_g | Glass Transition Temperature |
| T_m | Melting Temperature |
| TAAMP | Tris(azido acetoxy methyl) propane |
| TATB | 1,3,5-Triamino-2,4,6-trinitrobenzene |
| TDI | Toluene diisocyanate |
| TEGDN | Triethylene glycol dinitrate |
| TEX | 4,10-Dinitro-2,6,8,12-tetraoxa-4,10-diazaisowurtzitane |
| TFE | Tetrafluoroethylene |
| TGA | Thermogravimetric Analysis |
| THF | Tetrahydrofuran |
| TMETN | 1,1,1-Trimethylol ethane trinitrate |
| TMNTA | Trimethylol nitromethane tris(azido acetate) |
| TMP | Trimethylol propane |
| TNT | Trinitrotoluene |
| TNAZ | 1,3,3-Trinitroazetidine |
| TPB | Triphenyl bismuth |
| TPE | Thermoplastic Elastomer |
| TR | Technical Report |
| TTD | 2,2,4-Trifluoro-5-trifluoro-methoxy-1,3-dioxide |
| UK | United Kingdom |
| USA | United States of America |
| VDF | Vinylidene difluoride |
| Viton | Copolymer of vinylidene fluoride and hexafluoropropylene |
| VISAR | Velocity Interferometer System for Any Reflector |
| VOD | Velocity of Detonation |
| VTS | Vacuum Thermal Stability |

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