Electronic Supporting Information

Probing the Compatibility of Energetic Binder Poly Glycidyl Nitrate with Energetic Plasticizers: Thermal, Rheological and DFT Studies

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Cartesian coordinates of all the optimized stationary points at B3LYP/6-311G(d,p) in the gas phase, including corresponding charge and multiplicity were given below.

PGN2

Charge = 0; Multiplicity = 1

C	-0.95680600	0.90644800	-0.40536100
C	-1.11785200	2.10118200	0.53128800
H	-0.11836100	2.48090300	0.77355700
H	-1.60207100	1.76669900	1.45517900
O	-1.89784300	3.07090600	-0.15920400
H	-2.11226500	3.78051400	0.45198100
O	-0.11827300	-0.01398700	0.27333000
C	0.43742100	-1.04452100	-0.52839600
H	-0.31902700	-1.77460800	-0.83603400
H	0.91434600	-0.63145800	-1.42519300
C	1.47905300	-1.77502000	0.31381000
H	0.97671300	-2.15617400	1.21488400
C	2.59469400	-0.86081300	0.81343300
H	2.18121300	-0.09018600	1.46478600
H	3.34925600	-1.43046000	1.36288500
O	3.19944000	-0.25308900	-0.34717400
O	1.94997800	-2.83515100	-0.50365800
N	4.22115900	0.68739900	-0.04597000
O	4.68310600	1.19603700	-1.02659000
O	4.49560000	0.85478900	1.11815600
H	2.51355200	-3.40924800	0.02334800
C	-2.29772100	0.31348700	-0.83370900
H	-2.90112700	1.09535900	-1.29467000
H	-2.17349100	-0.51189200	-1.53685600
O	-2.94147800	-0.16801000	0.36687700
N	-4.26164200	-0.65165800	0.16402400
O	-4.69182200	-0.63724400	-0.96378400
O	-4.77724500	-1.02291900	1.17981100
H	-0.46979500	1.25513000	-1.32874900

BDNPA

Charge = 0; Multiplicity = 1

C	0.17798700	1.79187600	-0.80363500
H	0.17291000	1.70050600	-1.90396500
C	0.49957600	3.20088800	-0.35253700
H	-0.23414400	3.90468700	-0.74978500
H	0.48223000	3.23662300	0.73729400
H	1.49359600	3.49319200	-0.69612300
O	-1.08400100	1.45654100	-0.29999900
O	1.12561700	0.85822600	-0.28389400
C	-1.56539400	0.18294600	-0.70449300
H	-0.98191400	-0.62496500	-0.26117800
H	-1.55186000	0.08045500	-1.79490600
C	2.17278300	0.50906400	-1.15731400
H	1.78764100	0.00136300	-2.05051700
H	2.76656500	1.37637000	-1.46569800
C	-3.01142000	0.10516600	-0.22106700
C	3.10466500	-0.46279000	-0.44178700
N	-3.60012800	-1.27532100	-0.57107300
O	-3.01711100	-1.92990200	-1.41568300

O	-4.63487500	-1.57343300	-0.00945700
N	3.96202000	0.25566200	0.62838100
O	3.81553300	1.45573500	0.75726900
O	4.75323700	-0.44370800	1.22929700
C	4.03558300	-1.21066200	-1.38045700
H	4.71767400	-1.83927000	-0.81069800
H	3.44471800	-1.82979000	-2.05301600
H	4.61844000	-0.49498800	-1.96469300
N	2.19940400	-1.46802100	0.31946300
O	2.12004000	-1.38635500	1.52055500
O	1.59681200	-2.24018600	-0.40763600
C	-3.93571000	1.17300800	-0.76436700
H	-3.52921700	2.15124500	-0.51700400
H	-3.99764000	1.07222700	-1.85046700
H	-4.92885500	1.07231900	-0.33131800
N	-2.99056700	0.12194200	1.33235000
O	-2.37444000	-0.78660400	1.85491300
O	-3.56627200	1.03008800	1.89240600

BTTN

Charge = 0; Multiplicity = 1

C	2.07061900	-0.30711600	-0.35653400
C	0.80664800	-0.70079600	0.39962900
H	0.79210800	-1.78855800	0.51402400
H	0.82059800	-0.26667900	1.39907700
C	-0.46027100	-0.29374500	-0.35783900
H	-0.44612100	-0.74274800	-1.35486300
C	-1.73642500	-0.75941100	0.33469900
H	-1.91845300	-0.24286700	1.27445900
O	-0.48067100	1.11035000	-0.74624600
N	-0.55978800	2.09909000	0.29019200
O	-0.61428700	1.71744000	1.43545300
O	-0.55821900	3.20727100	-0.14982000
H	2.09458900	-0.74052400	-1.35974500
H	2.18050500	0.77450100	-0.44399400
O	3.15077300	-0.84664300	0.43307700
N	4.45090100	-0.56923200	-0.09561100
O	5.32539800	-1.02288000	0.58150800
O	4.50300500	0.06218000	-1.12165300
O	-2.80104400	-0.49627500	-0.59896600
N	-4.09037300	-0.91557700	-0.13433100
O	-4.95848500	-0.66833100	-0.91599300
O	-4.13510600	-1.44981500	0.94582500
H	-1.66275500	-1.83305600	0.52409400

BuNENA

Charge = 0; Multiplicity = 1

N	0.64160200	0.57277900	0.17074300
C	1.76045400	-0.14276600	0.79274500
H	1.32081900	-1.01205100	1.28877900
C	-0.45064900	-0.12364300	-0.49995300
H	-0.18693300	-1.18122400	-0.53574100
H	-0.55733900	0.24102300	-1.52189200
C	-1.76935500	0.05437600	0.25344300
H	-2.08836200	1.09577700	0.23749800

H	-1.68568200	-0.28981100	1.28644700
O	-2.70576900	-0.77107200	-0.46974000
N	0.81517200	1.90662400	-0.13332500
O	1.84201400	2.44448200	0.26182000
O	-0.08968100	2.45444400	-0.75647300
N	-4.03372700	-0.74193600	0.05466200
O	-4.22384500	-0.06069000	1.03102700
O	-4.78850600	-1.42603300	-0.57238500
C	2.85688000	-0.57261200	-0.18869600
H	3.25599500	0.31966400	-0.67964700
H	2.42170200	-1.20489800	-0.97188700
H	2.17433600	0.50299000	1.56643300
C	3.99165000	-1.32928900	0.51176300
H	4.41540600	-0.69359900	1.29772000
H	3.58399100	-2.21275300	1.01838400
C	5.10200300	-1.76007400	-0.45038400
H	5.55397500	-0.89462300	-0.94346700
H	5.89606600	-2.29541400	0.07609700
H	4.71508400	-2.42234500	-1.23077600

DEGDN

Charge = 0; Multiplicity = 1

C	-2.33930800	0.25851900	0.00001500
H	-2.31236700	0.88999900	-0.88940000
H	-2.31237100	0.88986400	0.88952600
C	-1.18267000	-0.72851800	-0.00003200
H	-1.23270600	-1.37048700	0.88950200
H	-1.23273100	-1.37049600	-0.88955900
O	-0.00000100	0.04970400	-0.00004300
C	1.18266900	-0.72851800	0.00005200
H	1.23272900	-1.37057800	-0.88941500
H	1.23270600	-1.37040400	0.88964600
C	2.33930700	0.25852000	-0.00002800
H	2.31235000	0.89002200	0.88937100
H	2.31238500	0.88984300	-0.88955500
O	3.52403600	-0.56248900	0.00007600
N	4.74344300	0.17876500	0.00001500
O	4.65518900	1.38143800	-0.00014300
O	5.70907600	-0.52758300	0.00006000
O	-3.52403700	-0.56249000	-0.00004600
N	-4.74344200	0.17876600	0.00013500
O	-4.65518600	1.38143900	0.00011500
O	-5.70907500	-0.52758100	-0.00017100

DNDA-57

Charge = 0; Multiplicity = 1

C	-0.18202700	-0.41643300	1.15377200
H	-0.42950100	0.31728500	1.91568700
H	0.03739100	-1.37523800	1.61698600
N	1.01421400	0.06775500	0.47811800
N	-1.35344400	-0.61846100	0.31896100
C	1.49112000	1.46113400	0.53143500
H	0.90846200	1.93666900	1.32017400
H	2.53819600	1.44267500	0.83812700
C	1.32717000	2.22564800	-0.78080200

H	1.71263400	3.24113500	-0.65601700
H	1.88966000	1.74657300	-1.58263400
H	0.27470900	2.29491900	-1.05878600
N	1.83265300	-0.87154900	-0.11044500
O	1.43907500	-2.03716100	-0.11339900
O	2.88718600	-0.47528800	-0.58477000
C	-1.68085800	-1.87137900	-0.35929600
H	-1.02288400	-2.63622700	0.04355700
H	-2.72438600	-2.13080700	-0.18116600
H	-1.51595700	-1.79207200	-1.43593000
N	-2.07536500	0.49570300	-0.04613900
O	-3.00371100	0.32131600	-0.82046500
O	-1.73844500	1.57202500	0.44687000

PGN2-PGN2

Charge = 0; Multiplicity = 1

C	2.59346700	-1.95690500	0.45734400
C	2.23251900	-2.98021800	-0.62843300
H	2.73565100	-2.69157900	-1.55715300
H	1.15848700	-2.96490100	-0.81364900
O	2.56987500	-4.30175800	-0.22399100
H	3.51505900	-4.42876400	-0.35053700
O	2.21134400	-0.68394900	-0.03172500
C	2.72434900	0.43699500	0.68731900
H	2.00983900	0.76248100	1.45255200
H	3.67177800	0.19101200	1.17683800
C	2.96684100	1.59579800	-0.28605100
H	2.02680200	1.83192800	-0.80349300
C	3.95612000	1.25369100	-1.38946000
H	3.52731400	0.52392300	-2.07657500
H	4.23378200	2.15955800	-1.92802500
O	5.12630600	0.68218200	-0.75560100
O	3.44960000	2.71953300	0.42934200
N	6.15084900	0.30281700	-1.65803200
O	7.08452300	-0.21014400	-1.10732300
O	5.97180100	0.52736900	-2.83054500
H	2.69556100	3.13246000	0.86896700
C	1.99435000	-2.30071500	1.82026700
H	2.29812600	-3.30874800	2.10310100
H	2.30263400	-1.59053700	2.58842500
O	0.54924800	-2.25285600	1.68919700
N	-0.15843300	-2.54917700	2.88730300
O	0.48604700	-2.78812900	3.87278600
O	-1.35036700	-2.51271600	2.73172600
H	3.68500100	-1.98007200	0.61393500
C	-2.78123700	-0.53588800	-0.02504500
C	-1.58187600	-0.97979300	-0.87436100
H	-0.70852400	-0.38537700	-0.58717500
H	-1.79733400	-0.79416400	-1.92710000
O	-1.33534100	-2.37188800	-0.73785500
H	-0.93278500	-2.51409400	0.12704300
O	-2.93543600	0.86590400	-0.22850600
C	-3.55416200	1.56850100	0.83553900
H	-4.55716200	1.18551200	1.05474900
H	-2.95286200	1.50717400	1.75096300

C	-3.68388900	3.03018100	0.41434600
H	-4.37275300	3.08195700	-0.44076300
C	-2.36651600	3.61321600	-0.08750700
H	-2.03146100	3.06671700	-0.96691700
H	-2.46002900	4.67669800	-0.32141100
O	-1.39525200	3.45360900	0.98174200
O	-4.20470300	3.71229800	1.54398900
N	-0.06778300	3.58566400	0.58313600
O	0.71316900	3.37804100	1.48417600
O	0.16622500	3.87845400	-0.56408200
H	-4.54986600	4.56533800	1.26478300
C	-4.05192900	-1.31503100	-0.35052500
H	-3.86598700	-2.38152400	-0.22219300
H	-4.89003700	-1.01411700	0.28106200
O	-4.36488700	-1.03030300	-1.73230600
N	-5.47472700	-1.75541000	-2.23826400
O	-6.04716200	-2.49880600	-1.47831400
O	-5.69817600	-1.51159100	-3.38998300
H	-2.55332900	-0.73913500	1.03117000

PGN-BDNPA

Charge = 0; Multiplicity = 1

C	-4.24098800	-0.03464900	0.34282600
C	-4.13379900	0.45256600	1.79415500
H	-3.14156000	0.18395500	2.16959500
H	-4.88440100	-0.05569500	2.40077700
O	-4.38410900	1.84425900	1.89031300
H	-3.59764200	2.31092700	1.58005900
O	-3.88322200	-1.40922900	0.35074100
C	-3.71606400	-2.01177000	-0.92001000
H	-4.67620600	-2.20066200	-1.41207700
H	-3.10095900	-1.38611500	-1.57880200
C	-3.02696800	-3.35643200	-0.70359000
H	-3.66442900	-3.95634700	-0.03896600
C	-1.68481100	-3.23269700	0.01351600
H	-1.82050400	-2.79801000	1.00386600
H	-1.19093300	-4.20289300	0.09720200
O	-0.86031800	-2.34881100	-0.79221500
O	-2.90928700	-3.94710900	-1.98813900
N	0.42257900	-2.13472100	-0.29336500
O	1.07049800	-1.37434900	-0.97012200
O	0.74723900	-2.71121700	0.71887000
H	-2.75283300	-4.89050900	-1.88765100
C	-5.61629900	0.24555400	-0.25830200
H	-5.84919200	1.30072500	-0.11191100
H	-5.66428500	0.00773300	-1.32264700
O	-6.55971200	-0.57838700	0.46169600
N	-7.91772100	-0.34484500	0.11367100
O	-8.13918900	0.48242400	-0.73697500
O	-8.67683400	-1.03340900	0.73395100
H	-3.52168100	0.53159200	-0.27113800
C	3.52019700	1.62923800	-1.27838300
H	3.00575300	0.98662500	-2.00946200
C	4.59893000	2.47352400	-1.92224200
H	4.16776900	3.11334900	-2.69408500

H	5.07240600	3.09511300	-1.16082500
H	5.35883000	1.83601600	-2.37795500
O	2.59117200	2.50182300	-0.68577000
O	4.05024500	0.79739700	-0.24467100
C	1.47301600	1.85165200	-0.10692300
H	1.74190300	1.33742700	0.81753900
H	1.02743600	1.12968900	-0.79616900
C	4.42038300	-0.50531100	-0.66989600
H	3.55244400	-1.08070600	-1.00198000
H	5.16658800	-0.47703800	-1.46779600
C	0.46749400	2.95525900	0.20865700
C	5.03220300	-1.18663100	0.55033900
N	-0.83223400	2.32511500	0.73955000
O	-0.81562200	1.14708000	1.03823500
O	-1.78704800	3.07791600	0.84950700
N	5.58013200	-2.57098100	0.14977900
O	6.29784500	-3.11697300	0.96375000
O	5.22204000	-3.02394400	-0.92167900
N	6.30687400	-0.38540700	0.94076800
O	7.14655300	-0.28198200	0.06452700
O	6.36346600	0.08043800	2.05738700
N	0.03064900	3.59312100	-1.14206400
O	-0.52360500	2.83526000	-1.91825000
O	0.29039000	4.76050200	-1.32344200
C	4.10714300	-1.35175000	1.73491300
H	3.24546300	-1.95362100	1.43905100
H	4.63037300	-1.83096100	2.56002000
H	3.76380900	-0.36818800	2.04956800
C	0.94399000	4.00728400	1.18436900
H	0.19545800	4.78732300	1.30810300
H	1.14803100	3.53566900	2.14821500
H	1.86581400	4.44009300	0.80083100

PGN-BTTN

Charge = 0; Multiplicity = 1

C	4.60782400	-0.20662200	-1.08630800
C	3.16490300	-0.70329800	-1.18499300
H	2.53125800	0.11908300	-1.53961900
H	2.82236700	-0.99879000	-0.18728900
O	3.15192200	-1.79567000	-2.09199400
H	2.24578200	-2.12207300	-2.13720900
O	4.67712900	0.95278700	-0.25872000
C	4.43496500	2.18365700	-0.92289500
H	5.34070000	2.54510200	-1.42411400
H	3.63887400	2.09597900	-1.66847100
C	4.00790900	3.20814300	0.12616300
H	4.83460100	3.34160500	0.83892000
C	2.81938200	2.73371800	0.96029500
H	3.09845600	1.85868400	1.54668500
H	2.45911500	3.52462600	1.62249800
O	1.76782400	2.37481400	0.02829500
O	3.74564900	4.40399300	-0.59143500
N	0.64684000	1.77260800	0.61767000
O	-0.16066800	1.39901900	-0.19738100
O	0.60721400	1.69584800	1.81999900

H	3.68106100	5.13493600	0.03010000
C	5.55903800	-1.25343600	-0.53211200
H	5.53707300	-2.13985900	-1.16569800
H	6.57367700	-0.85761000	-0.46748300
O	5.08733800	-1.58717100	0.79442400
N	5.80536100	-2.63742500	1.41703200
O	6.72449000	-3.12486000	0.80362200
O	5.38556200	-2.90059300	2.50863600
H	4.96720700	0.02151000	-2.09950500
C	-5.98481000	-1.04989700	-0.85383300
H	-6.55298300	-1.73855300	-1.48125900
H	-6.04519800	-0.04684500	-1.27726900
C	-4.54347900	-1.50997300	-0.70461400
H	-4.52179400	-2.49429400	-0.22817700
H	-4.11050900	-1.61993700	-1.70126000
C	-3.68023500	-0.55553100	0.12391500
H	-4.15889700	-0.35040600	1.08278200
C	-2.28002400	-1.07565300	0.41485500
H	-1.66529400	-0.30605300	0.87564900
O	-6.53374400	-1.04967500	0.48600700
O	-3.63124000	0.67034100	-0.64672200
N	-3.36087000	1.86487200	0.10991800
O	-3.20926500	1.74576900	1.29968500
O	-3.33275500	2.83643900	-0.58141300
N	-7.89119200	-0.60997800	0.56572800
O	-8.30454800	-0.60343000	1.68800300
O	-8.43389900	-0.31504900	-0.46947500
H	-2.32906900	-1.94874500	1.07038700
O	-1.70872100	-1.45514700	-0.86154900
N	-0.34779500	-1.79403600	-0.80446400
O	0.18631800	-1.80833700	0.27594600
O	0.11318500	-2.04123700	-1.89013800

PGN-BuNENA

Charge = 0; Multiplicity = 1

C	-3.42995500	-0.42350900	-0.12390600
C	-3.11873700	-1.13215700	-1.44956500
H	-2.15471800	-0.76194100	-1.81619300
H	-3.88317000	-0.88287900	-2.18656600
O	-3.12468800	-2.54002900	-1.29184200
H	-2.29640300	-2.78642300	-0.86225500
O	-3.25706500	0.97048300	-0.34714000
C	-3.08291000	1.75627700	0.81821000
H	-4.02147100	1.89246600	1.36692800
H	-2.34854900	1.30138000	1.49419300
C	-2.57782200	3.13128100	0.38743900
H	-3.36083200	3.61478100	-0.21304000
C	-1.35078700	3.06118300	-0.51912800
H	-1.60534000	2.58969000	-1.46828100
H	-0.93897500	4.05655800	-0.69629000
O	-0.36296200	2.24873500	0.16631100
O	-2.33138600	3.84459400	1.59026700
N	0.84110400	2.09103800	-0.52902900
O	1.60560500	1.34026800	0.02854800
O	0.98863300	2.69369600	-1.56248700

H	-2.34184000	4.78762000	1.40357900
C	-4.80962700	-0.78544800	0.41833100
H	-4.88635100	-1.87119000	0.48742200
H	-4.99779500	-0.34546600	1.39954600
O	-5.77386400	-0.27688500	-0.53020900
N	-7.11775400	-0.62971800	-0.23814600
O	-7.31799500	-1.28093500	0.75855000
O	-7.89159900	-0.20871600	-1.05030000
H	-2.70966800	-0.76980800	0.63252800
N	4.49702400	-1.18266300	-0.14717300
C	4.92204500	0.11851700	-0.67634800
H	4.01583000	0.72485700	-0.73811600
C	3.46936700	-1.31206100	0.87759700
H	3.26314800	-0.31387200	1.26214300
H	3.83102700	-1.94045700	1.69135600
C	2.19017900	-1.90020400	0.28411600
H	2.34204400	-2.92309600	-0.05821500
H	1.81556300	-1.27654700	-0.52606100
O	1.24064100	-1.88556300	1.38381300
N	5.29103600	-2.28092800	-0.38626700
O	6.26720100	-2.12364000	-1.10890600
O	4.94139300	-3.34075900	0.12900000
N	-0.07189400	-2.19486100	1.02716700
O	-0.28460500	-2.49336200	-0.13247700
O	-0.84692300	-2.11905700	1.93959000
C	5.99085800	0.81712300	0.17165700
H	6.87381200	0.17364700	0.22618100
H	5.61910300	0.94388700	1.19558900
H	5.28734700	-0.04326100	-1.69017200
C	6.37906100	2.18309000	-0.40610100
H	6.74004300	2.05004700	-1.43259300
H	5.48650000	2.81664500	-0.47501100
C	7.45046900	2.89741800	0.42209500
H	8.36682600	2.30262800	0.47863000
H	7.70853900	3.86539100	-0.01491600
H	7.10680900	3.07556400	1.44562900

PGN-DEGDN

Charge = 0; Multiplicity = 1

C	1.50657400	2.35635000	0.72356800
C	2.53377200	2.69897700	-0.36385400
H	2.01579200	3.20636700	-1.18455700
H	2.97837600	1.78551800	-0.75884600
O	3.59918300	3.47831000	0.16521200
H	3.29881700	4.38788300	0.25497000
O	0.44730400	1.66686300	0.08159500
C	-0.66424300	1.34771000	0.90753900
H	-0.43774900	0.50695000	1.57126600
H	-0.96368000	2.20896100	1.51639000
C	-1.81971400	0.93086800	0.00188600
H	-1.45357100	0.12953600	-0.65565900
C	-2.29794000	2.04727500	-0.92037700
H	-1.49338100	2.33795200	-1.59762700
H	-3.16260100	1.72660800	-1.50746400
O	-2.66660300	3.16487900	-0.08518300

O	-2.82869800	0.45329300	0.88197600
N	-3.09117400	4.31557900	-0.80607700
O	-3.35792900	5.23560900	-0.08803100
O	-3.13166300	4.23117200	-2.00959600
H	-3.57579800	0.11299600	0.37643200
C	2.13418800	1.59172400	1.88967900
H	3.03161000	2.12037100	2.21246300
H	1.44936300	1.48526600	2.73235900
O	2.48022000	0.27986400	1.38878800
N	3.11279600	-0.56308600	2.34355500
O	3.33253400	-0.10146300	3.43389700
O	3.34213000	-1.65753700	1.90769500
H	1.12806200	3.29702600	1.15920500
C	-2.45941100	-2.72568600	-0.20841100
H	-2.70579700	-2.42180000	-1.22788500
H	-2.43028300	-1.85138000	0.44086000
C	-1.12022600	-3.44304900	-0.18815300
H	-0.85265100	-3.73189800	0.83632500
H	-1.15184500	-4.34915200	-0.80742700
O	-0.20568200	-2.49667100	-0.71231000
C	1.14206700	-2.94467600	-0.74699200
H	1.23170900	-3.86298500	-1.34170900
H	1.51870000	-3.14073000	0.26363200
C	1.93238700	-1.81524100	-1.38755000
H	1.89168700	-0.91950400	-0.77009600
H	1.55022200	-1.59352200	-2.38603400
O	3.28457100	-2.31031800	-1.47339100
N	4.21957000	-1.35414100	-1.94483300
O	3.79435000	-0.26276100	-2.24418600
O	5.33645300	-1.78128600	-1.98906800
O	-3.44386500	-3.66173200	0.27542700
N	-4.74591800	-3.10522900	0.37510500
O	-4.88411900	-1.94801500	0.04313000
O	-5.55551400	-3.88418600	0.78093400

PGN-DNDA-57

Charge = 0; Multiplicity = 1

C	2.50430900	-0.62432000	0.02294400
C	1.87017400	-1.40223100	1.18340100
H	1.00535800	-0.83271400	1.53727200
H	2.58973400	-1.48862800	1.99902900
O	1.51848300	-2.71454800	0.78387500
H	0.71543500	-2.65123700	0.24766300
O	2.71168700	0.70394900	0.48322700
C	3.08496300	1.64958600	-0.50246500
H	4.15447400	1.59637100	-0.73389500
H	2.51745900	1.50319700	-1.42968200
C	2.78306600	3.03946400	0.05310700
H	3.37643300	3.17683700	0.96829000
C	1.32515800	3.19380900	0.47867100
H	1.09276800	2.48524000	1.27197000
H	1.11171100	4.21203700	0.81385700
O	0.51258900	2.89993800	-0.68731000
O	3.16911900	3.95700600	-0.95871300
N	-0.85202700	2.75023900	-0.42569500

O	-1.48698900	2.45471300	-1.40583000
O	-1.23997900	2.93247900	0.70469700
H	3.24194700	4.83521300	-0.57403000
C	3.76755700	-1.29819700	-0.50529800
H	3.53596000	-2.33928100	-0.73244400
H	4.15932200	-0.80801000	-1.39883500
O	4.75241100	-1.22583600	0.55056900
N	5.95675300	-1.92065800	0.26880200
O	6.04591200	-2.46954500	-0.80321500
O	6.74783000	-1.85627600	1.16677600
H	1.79068100	-0.61770500	-0.81622400
C	-3.68179900	-0.10966900	-0.99117500
H	-3.05906100	0.78083300	-1.00133400
H	-4.38404100	-0.07808900	-1.82100500
N	-4.41000100	-0.11687800	0.26263100
N	-2.83606000	-1.27991100	-1.22894900
C	-4.10092100	0.76139100	1.40667900
H	-3.36993500	1.47956800	1.03717800
H	-5.01296600	1.30202200	1.66573600
C	-3.55121600	0.02021400	2.62337400
H	-3.34174900	0.74157700	3.41758300
H	-4.27570100	-0.70104200	3.00240400
H	-2.62060300	-0.49227000	2.37575700
N	-5.58530200	-0.83660800	0.29703800
O	-5.85176300	-1.51917900	-0.69187500
O	-6.26898800	-0.74564100	1.30483700
C	-3.19997700	-2.40634200	-2.08920800
H	-4.22431800	-2.24167000	-2.40914500
H	-2.52786400	-2.46672800	-2.94716800
H	-3.14595200	-3.34151500	-1.53136000
N	-1.61569500	-1.31196700	-0.63939600
O	-0.89986200	-2.28470100	-0.89504200
O	-1.30303100	-0.38057800	0.10265100

PGN-BDNPA-PGN

Charge = -1; Multiplicity = 1

C	-6.88518400	-0.74789600	-0.50301300
C	-6.60540600	-1.07500600	-1.97707900
H	-5.71812300	-0.51461900	-2.28863700
H	-7.45236000	-0.74913000	-2.58226700
O	-6.45345500	-2.46929600	-2.17859700
H	-5.57786600	-2.72042600	-1.85788300
O	-6.96039900	0.66882700	-0.41267200
C	-6.92776200	1.20731900	0.89703800
H	-7.83811600	0.97466700	1.46013900
H	-6.06385000	0.83166200	1.45948100
C	-6.83791300	2.72518800	0.76323900
H	-7.72499400	3.06482200	0.21060700
C	-5.63972700	3.18603900	-0.06270200
H	-5.70099800	2.79034300	-1.07651800
H	-5.57455000	4.27548800	-0.08972100
O	-4.45330600	2.65678100	0.58913900
O	-6.81883600	3.23682100	2.08667500
N	-3.25176800	3.00798400	-0.01832000
O	-2.28878500	2.52031900	0.52682700
O	-3.28258700	3.73415200	-0.98225700

H	-7.07719100	4.16279100	2.06889500
C	-8.12838000	-1.46321400	0.02013700
H	-8.03092500	-2.52847200	-0.19072300
H	-8.27521300	-1.31758300	1.09194400
O	-9.25474400	-0.91344600	-0.69888000
N	-10.48809000	-1.56477100	-0.43130800
O	-10.47583600	-2.47624200	0.36014200
O	-11.40095500	-1.09391900	-1.04832400
H	-6.04533300	-1.11557200	0.10814000
C	0.38116800	0.33439600	1.80290900
H	-0.43623800	0.94868300	2.21124300
C	1.39227000	-0.05228600	2.86154800
H	0.89989000	-0.60831400	3.66111700
H	2.16012700	-0.68421600	2.41326000
H	1.85786900	0.83689200	3.29131700
O	-0.13468100	-0.84851500	1.26249100
O	0.98485400	1.07073300	0.72805400
C	-1.16320900	-0.67319400	0.30396200
H	-0.76299000	-0.36155700	-0.66242400
H	-1.90252400	0.05922500	0.63752100
C	1.04665700	2.46832500	0.94000800
H	0.06390900	2.88741300	1.17105000
H	1.74902600	2.73225400	1.73560800
C	-1.81784100	-2.04460100	0.15187200
C	1.53171000	3.07935000	-0.37345200
N	-3.01961700	-1.93428300	-0.80136000
O	-3.12746000	-0.92648200	-1.47129800
O	-3.77079600	-2.89733200	-0.83095600
N	1.77335900	4.59273500	-0.18817800
O	2.41792400	5.13962800	-1.06010600
O	1.26263400	5.11995000	0.78125000
N	2.94860300	2.51380800	-0.65336300
O	3.79157400	2.76230400	0.19976900
O	3.12069300	1.86448300	-1.65800600
N	-2.47962400	-2.39873900	1.51567900
O	-3.35035600	-1.62886400	1.88790700
O	-2.07525200	-3.37396800	2.10376600
C	0.62389900	2.87496200	-1.56520800
H	-0.34907300	3.31962400	-1.35030100
H	1.05429800	3.33173300	-2.45461800
H	0.49486800	1.80764200	-1.73135600
C	-0.90402600	-3.15103000	-0.32271800
H	-1.43098000	-4.10320500	-0.33724800
H	-0.54555700	-2.91380000	-1.32684100
H	-0.04595700	-3.21013700	0.34451000
C	6.99484800	0.08745800	-0.08069000
C	6.61655400	1.01996500	-1.23956300
H	5.65284200	0.69735800	-1.64561000
H	7.36858400	0.93193400	-2.02531400
O	6.59007400	2.37231600	-0.81853200
H	5.72761600	2.54371700	-0.41898400
O	6.92595600	-1.23693200	-0.58930200
C	7.12547300	-2.27452100	0.35413100
H	8.17431200	-2.35005000	0.66004500
H	6.50801800	-2.12439000	1.24871800

C	6.73899900	-3.58777800	-0.32008000
H	7.36498800	-3.69874300	-1.21678500
C	5.29573400	-3.60593200	-0.81746600
H	5.14296100	-2.82523400	-1.56328000
H	5.03973200	-4.57845200	-1.24350100
O	4.45164200	-3.35136200	0.33267400
O	7.00591200	-4.60640300	0.63128700
N	3.07416800	-3.38660600	0.06478700
O	2.40322900	-3.15208100	1.03525100
O	2.72241500	-3.64265100	-1.06351600
H	7.01699100	-5.45765700	0.18423800
C	8.34762300	0.45277100	0.52715800
H	8.34033100	1.51603000	0.76823600
H	8.57283300	-0.12248900	1.42730900
O	9.34527000	0.17578000	-0.48098000
N	10.65601400	0.59853900	-0.13170500
O	10.80461400	1.11331000	0.95006500
O	11.45839500	0.36892700	-0.99120600
H	6.25750900	0.21453400	0.72948100

PGN-BTTN-PGN

Charge = 0; Multiplicity = 1

C	-7.58315700	1.20946500	-0.25884400
C	-6.14675200	1.06863100	-0.76341700
H	-5.92760400	-0.00093300	-0.87266300
H	-5.46224200	1.47632600	-0.00685600
O	-6.03432000	1.75461900	-1.99887300
H	-5.14332600	1.60042600	-2.33396300
O	-7.71953200	0.47375100	0.95755900
C	-8.22954400	-0.84251400	0.80615600
H	-9.31703600	-0.82784300	0.67393700
H	-7.78051000	-1.35530000	-0.05079500
C	-7.89234400	-1.62982100	2.07004100
H	-8.41221600	-1.16537500	2.92015300
C	-6.40530500	-1.57772300	2.41801400
H	-6.11490600	-0.55997200	2.67587400
H	-6.16792100	-2.25138300	3.24481100
O	-5.67914600	-1.99879300	1.23533800
O	-8.36082600	-2.94882200	1.83528000
N	-4.28892000	-1.83717000	1.31614700
O	-3.72936800	-2.10447800	0.28146900
O	-3.81780400	-1.46513300	2.36238900
H	-8.41801400	-3.41506500	2.67423200
C	-7.92327600	2.66073400	0.01677500
H	-7.41871300	3.00693600	0.92076900
H	-7.63801000	3.28236900	-0.83194900
O	-9.35634100	2.70296500	0.20985900
N	-9.86195800	3.98940400	0.52277300
O	-9.06854400	4.89739900	0.59431600
O	-11.05055200	3.99432200	0.67864400
H	-8.27001900	0.82588700	-1.02169900
C	2.18981200	-2.48263900	-2.33683300
H	2.74973700	-2.19352000	-3.22546000
H	1.82315100	-3.50382100	-2.44459900
C	1.06996500	-1.49565400	-2.05857000

H	1.49302500	-0.49758700	-1.92523100
H	0.42333900	-1.46111300	-2.93825100
C	0.23343300	-1.83799900	-0.82515900
H	0.87960200	-2.00123400	0.03885700
C	-0.76802400	-0.75830200	-0.44233800
H	-1.43423600	-1.09708700	0.34796900
O	3.07059000	-2.41025100	-1.17913800
O	-0.43368500	-3.08298900	-1.15055900
N	-0.84138000	-3.87860800	-0.02305800
O	-0.58862900	-3.45400700	1.07683500
O	-1.38484900	-4.88637900	-0.35771700
N	4.20782300	-3.23349100	-1.25947300
O	4.91281900	-3.14057800	-0.28416900
O	4.34885200	-3.91092600	-2.24300400
H	-0.24066800	0.14316000	-0.12162500
O	-1.53948200	-0.47212200	-1.63640000
N	-2.58749200	0.43514700	-1.43897200
O	-2.71378900	0.92577600	-0.34410700
O	-3.24170300	0.61258500	-2.43577100
C	7.74478000	0.53910000	0.66416600
C	6.82849100	-0.58689700	0.18370600
H	6.57858500	-0.39498700	-0.86841100
H	5.89445000	-0.55941700	0.76128500
O	7.51273700	-1.81688500	0.34690500
H	6.89630800	-2.52679400	0.13468100
O	7.09587900	1.78965700	0.43059700
C	7.53244200	2.48476100	-0.72750100
H	8.51580400	2.93951000	-0.56555300
H	7.59142700	1.82314400	-1.59832400
C	6.51786700	3.58615400	-1.02419700
H	6.52463600	4.30049100	-0.18909500
C	5.08633300	3.05823900	-1.10453800
H	4.77430300	2.67039900	-0.13582500
H	4.39433900	3.83514600	-1.43729000
O	5.09190600	1.97795900	-2.07423100
O	6.94985200	4.19481500	-2.23139500
N	3.90361400	1.24462900	-2.14322700
O	3.97371600	0.30478700	-2.89099900
O	2.96511700	1.61682400	-1.47401700
H	6.56177600	5.07191400	-2.29768800
C	8.03594600	0.41330100	2.14696300
H	7.15613000	0.68408900	2.73361300
H	8.34645600	-0.60402500	2.38528800
O	9.10965500	1.34351300	2.41799000
N	9.48471600	1.41670400	3.78420900
O	8.88963900	0.71109400	4.56270900
O	10.37188500	2.19873200	3.97850100
H	8.69090700	0.48685600	0.11438600

PGN-BuNENA-PGN

Charge = 0; Multiplicity = 1

C	6.56011700	-1.27211000	0.41523500
C	5.77997900	-1.75235200	1.64695300
H	4.96115900	-1.04686000	1.82746300
H	6.43369100	-1.74799900	2.51996200

O	5.31384800	-3.07903900	1.47379200
H	4.54444500	-3.04250300	0.89290900
O	6.85209900	0.10473100	0.61980000
C	7.18478500	0.83586900	-0.54679600
H	8.19516600	0.60546300	-0.90256400
H	6.47592200	0.62809400	-1.35771800
C	7.12408100	2.32305800	-0.20572400
H	7.91383800	2.54479100	0.52530700
C	5.81559500	2.72801600	0.46982700
H	5.73214300	2.25963300	1.45045900
H	5.74496800	3.81295000	0.56707000
O	4.73616200	2.25163500	-0.37677000
O	7.34378100	3.00698200	-1.43032100
N	3.45567800	2.54253900	0.09958900
O	2.58362600	2.04981100	-0.57780700
O	3.35146900	3.22434000	1.08771100
H	7.65589800	3.89654300	-1.24172400
C	7.79813800	-2.12185700	0.14393700
H	7.49881300	-3.16833800	0.07368500
H	8.30777100	-1.82846300	-0.77588400
O	8.68503400	-1.93106300	1.26821900
N	9.85027800	-2.74323900	1.23237200
O	9.98838900	-3.47513400	0.28238600
O	10.55891400	-2.57401600	2.18328300
H	5.91584400	-1.38693900	-0.46975600
N	-1.02362200	0.83572300	-0.97467900
C	-0.97717200	2.20324800	-0.42756600
H	0.07301900	2.38784000	-0.19354000
C	0.04615200	0.28684900	-1.80264200
H	0.66274900	1.12544400	-2.12310400
H	-0.37973300	-0.20013900	-2.67915000
C	0.90373100	-0.69786000	-1.00788300
H	0.34004900	-1.58546900	-0.72223200
H	1.33308300	-0.21820100	-0.12981400
O	1.96359600	-1.06313100	-1.92741300
N	-2.16861800	0.12090900	-0.86312900
O	-3.11909600	0.63316200	-0.27796300
O	-2.17260400	-1.01916600	-1.35129300
N	3.01410700	-1.78622400	-1.35036100
O	2.91214700	-2.08132500	-0.17587300
O	3.90530100	-2.02327000	-2.11519800
C	-1.52023400	3.26729000	-1.38729100
H	-2.56739700	3.04749600	-1.61229700
H	-0.96635200	3.22324800	-2.33278700
H	-1.54056900	2.20657600	0.50463900
C	-1.41132600	4.67460000	-0.78704000
H	-1.95671400	4.69785800	0.16163900
H	-0.36172500	4.89075800	-0.55272000
C	-1.96684700	5.75590400	-1.71713200
H	-3.02897500	5.58915100	-1.91390800
H	-1.86280400	6.74846700	-1.27152700
H	-1.44137100	5.76538300	-2.67729900
C	-6.81885400	0.28590000	1.91783900
C	-8.21767700	0.91320100	1.98021100
H	-8.96000000	0.11591800	1.86909500

H	-8.33745400	1.60781100	1.14852800
O	-8.40696000	1.66388300	3.17390100
H	-8.56885000	1.04876000	3.89569200
O	-6.76272600	-0.45197000	0.71387300
C	-5.70708400	-1.40632500	0.62112100
H	-4.73984600	-0.94811800	0.84370200
H	-5.87748400	-2.24200600	1.30989000
C	-5.65150900	-1.91136000	-0.82234000
H	-5.58126700	-1.02963500	-1.47451000
C	-6.91344200	-2.63892400	-1.25450600
H	-7.76980900	-1.96492200	-1.22180800
H	-6.78710900	-3.04178100	-2.25984100
O	-7.12051400	-3.72726000	-0.32122500
O	-4.54088300	-2.77163100	-0.99550000
N	-8.29671600	-4.47393600	-0.55327000
O	-8.45539200	-5.35230500	0.24844600
O	-8.98395600	-4.15745500	-1.49581700
H	-3.75024800	-2.22135100	-1.08859800
C	-5.70770800	1.32992300	2.03704500
H	-5.85697800	1.92116500	2.94157600
H	-4.71757900	0.87657700	2.04904400
O	-5.82192000	2.18178600	0.87105800
N	-4.79208600	3.12285400	0.73437600
O	-3.95585600	3.17889600	1.60819300
O	-4.88418400	3.77515100	-0.27040700
H	-6.69599200	-0.38489000	2.78575100

PGN-DEGDN-PGN

Charge = 0; Multiplicity = 1

C	-4.06069200	-3.01718000	-0.35775000
C	-3.79742400	-3.83144400	0.91659600
H	-4.45521900	-3.45944900	1.70908600
H	-2.76514900	-3.68894900	1.23671500
O	-3.96677900	-5.22372200	0.68441800
H	-4.90825400	-5.42193500	0.68023000
O	-3.93009700	-1.65247600	-0.00084200
C	-4.32847300	-0.71594100	-0.99394200
H	-3.56482800	-0.61051500	-1.77178100
H	-5.27311800	-1.01710300	-1.46133800
C	-4.50357400	0.64225000	-0.31938200
H	-3.55650500	0.89045900	0.18001300
C	-5.56832700	0.64085900	0.77258800
H	-5.27097100	-0.03068200	1.57921100
H	-5.71427400	1.64585600	1.17698400
O	-6.79656500	0.17552400	0.17379000
O	-4.78180000	1.54933500	-1.37726300
N	-7.88339700	0.06604800	1.08471300
O	-8.87681200	-0.35714300	0.56719000
O	-7.68426800	0.40008300	2.22746100
H	-4.82160200	2.45094000	-1.03746500
C	-3.15653600	-3.44906400	-1.51178800
H	-3.23676100	-4.52899800	-1.63669800
H	-3.41025800	-2.95072700	-2.44887100
O	-1.80592800	-3.09472300	-1.13304900
N	-0.80349300	-3.55612300	-2.02410500

O	-1.15732300	-4.18768300	-2.98556700
O	0.30094800	-3.23209300	-1.67733800
H	-5.09081400	-3.21651500	-0.69887200
C	-1.83075400	3.10328000	-0.92841900
H	-2.09581600	3.27102200	0.11728700
H	-2.61012000	2.52315500	-1.42095800
C	-0.50198500	2.37385400	-1.01886700
H	-0.21348000	2.22859300	-2.06812900
H	0.29287100	2.92944400	-0.50923800
O	-0.74611000	1.13185500	-0.37513200
C	0.40974300	0.32599800	-0.21889400
H	1.23628300	0.91585000	0.18832500
H	0.71718100	-0.11162700	-1.17750700
C	0.02106000	-0.77208900	0.75746200
H	-0.76477000	-1.40488900	0.35095600
H	-0.29138400	-0.34504400	1.71154400
O	1.23510700	-1.54462500	0.94590100
N	1.05152000	-2.74915200	1.64896900
O	-0.05297200	-3.01173500	2.04499300
O	2.07344800	-3.37704200	1.77598500
O	-1.66530400	4.36964100	-1.59985900
N	-2.85818000	5.13186600	-1.66045100
O	-3.85291500	4.65472600	-1.15751900
O	-2.71427600	6.18141500	-2.21351100
C	4.86652100	-0.64597300	0.21109200
C	5.11230700	-1.42619800	1.51034500
H	4.41414100	-1.05618600	2.26941300
H	6.12852000	-1.23146000	1.85695100
O	4.99064600	-2.82034900	1.30249600
H	4.05338600	-3.04981900	1.32988900
O	4.97851700	0.73501200	0.53803300
C	4.47955700	1.63669200	-0.43042600
H	5.06800600	1.61809600	-1.35450600
H	3.43653800	1.40806300	-0.68295000
C	4.55889200	3.04775600	0.14743700
H	5.61936300	3.30053200	0.28520700
C	3.92502400	3.17649800	1.53004200
H	4.43281300	2.52219500	2.23842300
H	3.96751600	4.20919700	1.88384400
O	2.53951500	2.77405000	1.40319100
O	3.94583200	3.88852200	-0.81993100
N	1.80759800	2.80623400	2.61484100
O	0.67148200	2.43535700	2.47715600
O	2.37781800	3.18891600	3.60387700
H	4.21746000	4.79778900	-0.66416200
C	5.80482200	-1.08530100	-0.90976800
H	5.73615200	-2.16813400	-1.01631500
H	5.56760900	-0.61123400	-1.86409300
O	7.13891700	-0.70665500	-0.50424100
N	8.16168700	-1.15866000	-1.38027700
O	7.82205700	-1.77877800	-2.35875800
O	9.25671900	-0.84074700	-1.01254100
H	3.84551000	-0.86670600	-0.13649600

PGN-DNDA-PGN

Charge = 0; Multiplicity = 1

C	6.05793100	-0.48556900	-0.75290700
C	5.38508200	-1.85722900	-0.89788100
H	4.66812200	-1.96887600	-0.07837400
H	6.13767500	-2.64229200	-0.81317200
O	4.76976000	-1.98904200	-2.16625500
H	3.94940300	-1.47568100	-2.14570100
O	6.53002500	-0.39602900	0.58460800
C	6.98494100	0.88009700	0.99608400
H	8.01593200	1.06771200	0.67632500
H	6.34464800	1.67805700	0.60102900
C	6.94314600	0.91419600	2.52190800
H	7.60383900	0.12004700	2.89808300
C	5.55709400	0.59484000	3.07596400
H	5.25930800	-0.41073900	2.78228800
H	5.53105900	0.68729100	4.16480900
O	4.64055300	1.55924900	2.49735600
O	7.41033200	2.20059400	2.89698600
N	3.29029800	1.29986000	2.74363300
O	2.55533700	2.09497400	2.21688200
O	3.01001600	0.34869400	3.43611900
H	7.61877000	2.19686100	3.83573900
C	7.14140500	-0.25528300	-1.80269600
H	6.71587100	-0.44268800	-2.78915100
H	7.54587700	0.75827500	-1.76609000
O	8.19736900	-1.20177500	-1.52596400
N	9.24297500	-1.20214500	-2.48647800
O	9.15808800	-0.41961700	-3.40216500
O	10.09747700	-2.00424400	-2.23789000
H	5.29547100	0.29003200	-0.92830900
C	-0.00397800	0.73965800	0.42889200
H	0.74518700	1.10624500	1.12525200
H	-0.76092500	1.50334000	0.26521400
N	-0.61651700	-0.43374500	1.04697700
N	0.61874200	0.49962100	-0.86604200
C	-0.09324300	-1.10669800	2.25478700
H	0.71104400	-0.46925200	2.61813300
H	-0.89043100	-1.11506500	3.00015700
C	0.42586500	-2.52037600	2.00096400
H	0.82220200	-2.92260000	2.93690300
H	-0.37106900	-3.18046800	1.65881100
H	1.23237700	-2.50857900	1.26732900
N	-1.84470600	-0.79860800	0.59203700
O	-2.29141400	-0.21560600	-0.39567800
O	-2.43183500	-1.69290900	1.20712100
C	0.03224000	0.88421900	-2.15273000
H	-0.82575300	1.51723700	-1.93746100
H	0.76952900	1.42969200	-2.74437600
H	-0.29324400	0.00314000	-2.70823700
N	1.82722100	-0.11949500	-0.88095700
O	2.34389900	-0.30885000	-1.98464900
O	2.32383700	-0.44566600	0.19798000
C	-6.08820200	-0.78716800	0.01337100
C	-5.39781800	-1.81762800	-0.89324300

H	-4.66935400	-1.28576200	-1.51252500
H	-6.13902400	-2.28196200	-1.54479800
O	-4.79733100	-2.84629700	-0.12772900
H	-4.02091700	-2.46772600	0.31040200
O	-6.54354600	0.26394500	-0.82600900
C	-6.97364000	1.44027300	-0.16563000
H	-7.99142900	1.33909000	0.22691800
H	-6.30264400	1.69705800	0.66366500
C	-6.96133700	2.57614400	-1.18621400
H	-7.66671100	2.32151500	-1.99036000
C	-5.60451300	2.73661100	-1.86612600
H	-5.35449300	1.82917700	-2.41264900
H	-5.59764300	3.59445500	-2.54386700
O	-4.62670700	2.95487400	-0.81656300
O	-7.37531500	3.73580600	-0.48091400
N	-3.29438400	2.85674600	-1.23418100
O	-2.50867300	2.99848500	-0.33209300
O	-3.07675900	2.65506100	-2.40526300
H	-7.60122400	4.42391500	-1.11353300
C	-7.18748200	-1.41053600	0.86959500
H	-6.77237900	-2.27322700	1.39180900
H	-7.60095400	-0.70862900	1.59685000
O	-8.23156900	-1.83163300	-0.03715100
N	-9.28884100	-2.54307400	0.58621800
O	-9.22416100	-2.70303400	1.78161100
O	-10.13164000	-2.89218900	-0.19085000
H	-5.33850300	-0.39530900	0.71968000

Interaction between plasticizers and one segment polymeric binder (PGN-2)

To examine the intermolecular interactions responsible for the resultant viscosity of binder/plasticizer blend, we have considered all the five energetic plasticizers viz. DNDA-57, BuNENA, DEGDN, BTTN and BDNPA. To emulate the PGN polymer, we have used its corresponding dimeric unit for computing interaction energies with plasticizers as mentioned earlier. We brought one dimeric segment of PGN and each individual plasticizer together based on the sights of interaction obtained from MESP and allowed them to optimize towards possible mode of interactions. The relative reactivity of plasticizers with PGN-2 was examined by computing interaction energies for the purpose of assessing their respective compatibility properties towards PGN. The computed optimized geometries accompanied with the corresponding interactions which were marked with dotted lines were depicted in Fig. S1.

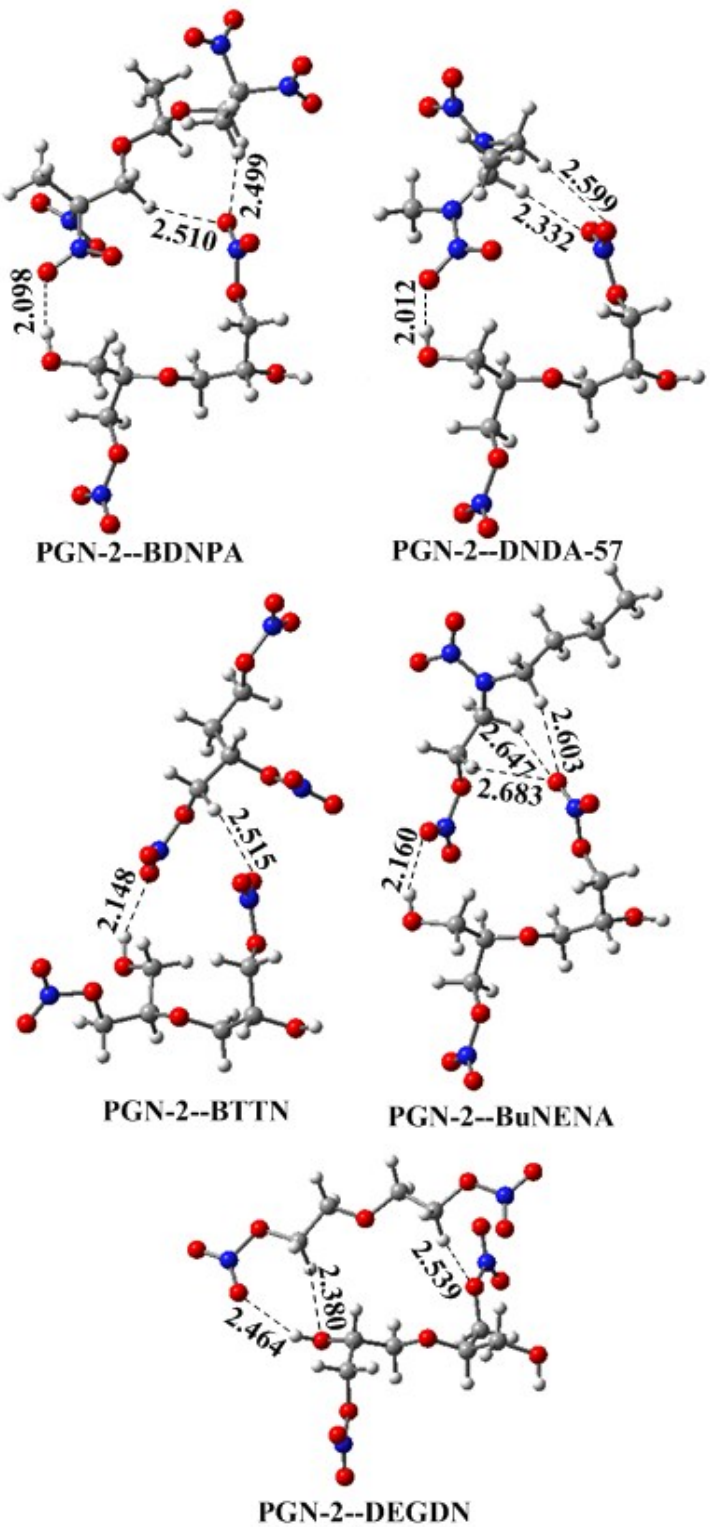


Fig. S1 Optimized geometries of adducts of one segment of PGN dimer and energetic plasticizer at B3LYP/6-311G(d,p) level. (grey: carbon; red: oxygen; blue: nitrogen; white: hydrogen).

In this study, the dimer of PGN forms a complex with BDNPA through two -C-H···O- type of interactions (2.510 Å and 2.499 Å) and one -O-H···O type of hydrogen bonding interaction at a distance of 2.098 Å. Complex of PGN-2 with DNDA-57 involves two -C-H···O- type of interactions (2.599 Å and 2.332 Å) and one -O-H···O (2.012 Å) type hydrogen bonding interaction. Complex of PGN-2 and BuNENA consist of one H-bond (2.160 Å) and three weak -C-H···O- type of interactions (2.603 Å, 2.647 Å and 2.683 Å). Similarly, the distances 2.380 Å and 2.539 Å are corresponding to -C-H···O- type of interactions whereas 2.464 Å is corresponding to -O-H···O kind of H-bonding in the case of DEGDN. Only two weak interactions: -C-H···O- (2.515 Å) and -O-H···O (2.148 Å) have been observed in the case of BTTN with PGN-2. The electronic interaction energies (kcal mol^{-1}) for the formation of the complex of PGN-2 with different plasticizers viz. BDNPA, BTTN, DNDA-57, BuNENA and DEGDN were found to be –14.3, –11.9, –11.6,–8.2 and –6.4, respectively (kcal/mol, Table 5 of main manuscript). The computed interaction energy results in terms of electronic and Gibbs free energies suggest that the monomer of BDNPA prefers to interact more strongly with PGN-2 whereas DEGDN has less interaction as compared to all other plasticizers. The interaction ability of plasticizers predicted using one segment of PGN-2 may not be sufficient as the plasticizer added to the binder system, plasticizer introduces between the polymeric segments of binder. Therefore, it is essential to consider at least two segments of polymeric binder.

Experimental

Caution: Some of the materials synthesized in the present investigation falls under the category of 1.1 HD. Therefore the materials must be synthesized and characterized by a skilled person with the knowledge of handling, storage and transport of energetic materials in accordance with the United Nations guidelines.

Characterization of GN and PGN:

The IR spectrum of glycidyl nitrate (Figure S2) showed stretching frequencies at 3008 & 2902 cm^{-1} (CH str.), 1647 &1281 cm^{-1} (-ONO2 str.), and 1135 cm^{-1} (C-O-C str.), respectively. The ^{1}H NMR spectrum of glycidyl nitrate (Figure S3) showed chemical shift at δ 2.73 & 2.91 (d, 2H, $-OCH_2$) and δ 3.27 (H, -O-CH), δ 4.35 & 4.74 (2H, CH_2ONO_2) respectively, whereas, the ^{13}C NMR spectrum of glycidyl nitrate (Figure S4) showed chemical shifts at δ 44.3, 47.5 and 73 corresponding to OCH_2 , CH and CH_2ONO_2, respectively. The IR spectra of PGN (Figure S5) showed stretching frequencies at 3469 cm^{-1} (OH), 2894 cm^{-1} (CH str.), 1633 & 1292 cm^{-1}($-ONO_2$ str.), and 1121 cm^{-1} (C-O-C str.),

respectively. The ^{1}H NMR spectrum of PGN (Figure S6) showed resonance at 4.5 ppm ($-CH_2ONO_2$), 3.6-3.77 ppm (O-CH_2 & C-H proton at the chiral center) and 3.1 ppm (-OH), whereas, the ^{13}C NMR of PGN (Figure S7) showed chemical shifts at δ 60.7, 64.4, and 68 corresponding to $-OCH_2-$, $-CH_2ONO_2$, and –OCH- respectively. The spectroscopic data obtained in the present investigation matches well with the reported data.[1-2]

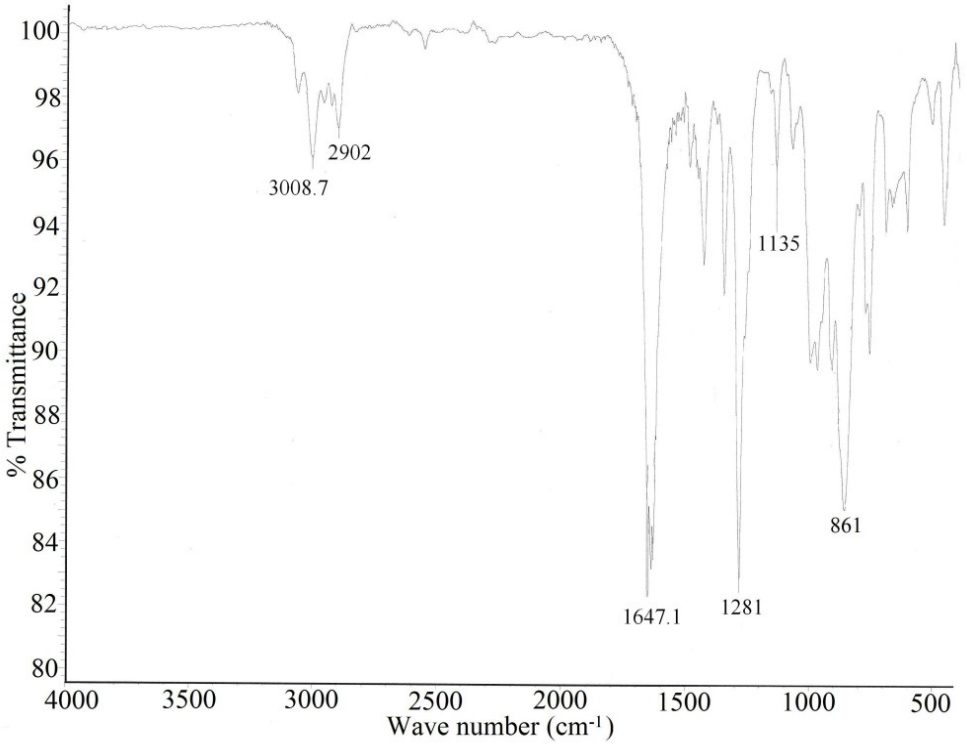


Fig. S2 IR Spectrum of GN

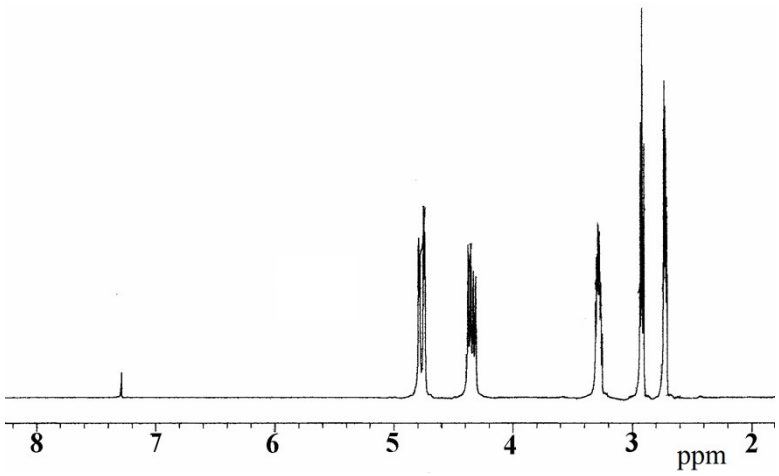


Fig. S3 ^{1}H NMR spectrum of GN

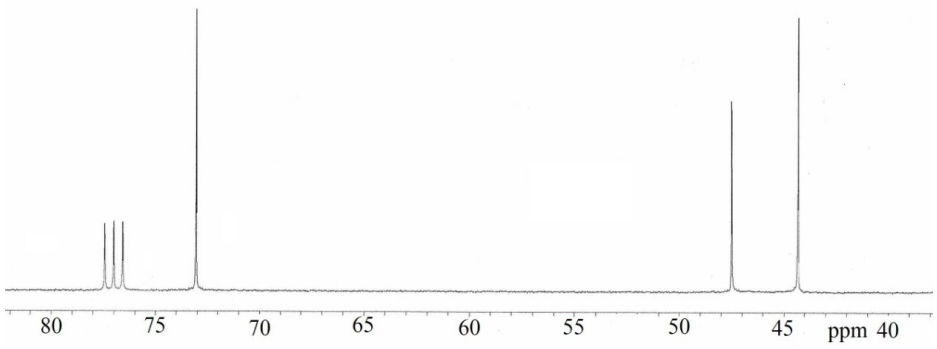


Fig. S4 ^{13}C NMR spectrum of GN

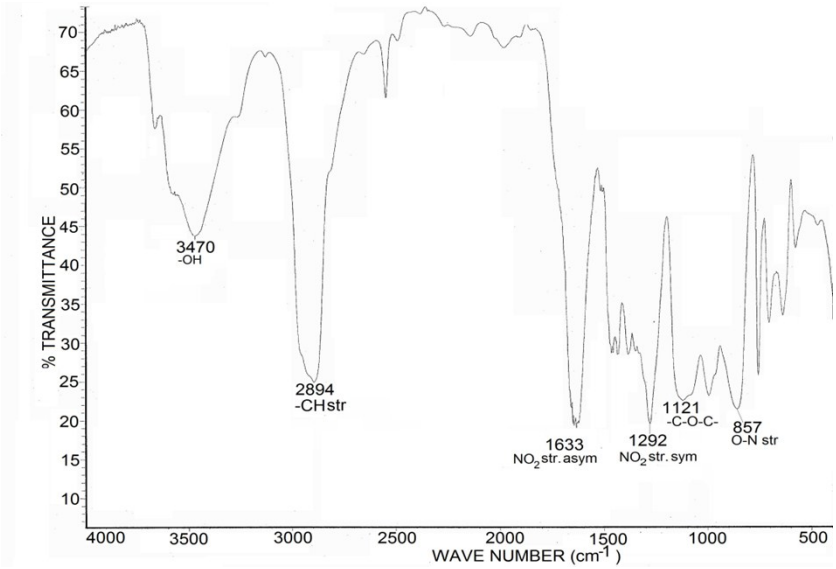


Fig. S5 IR Spectrum of PGN

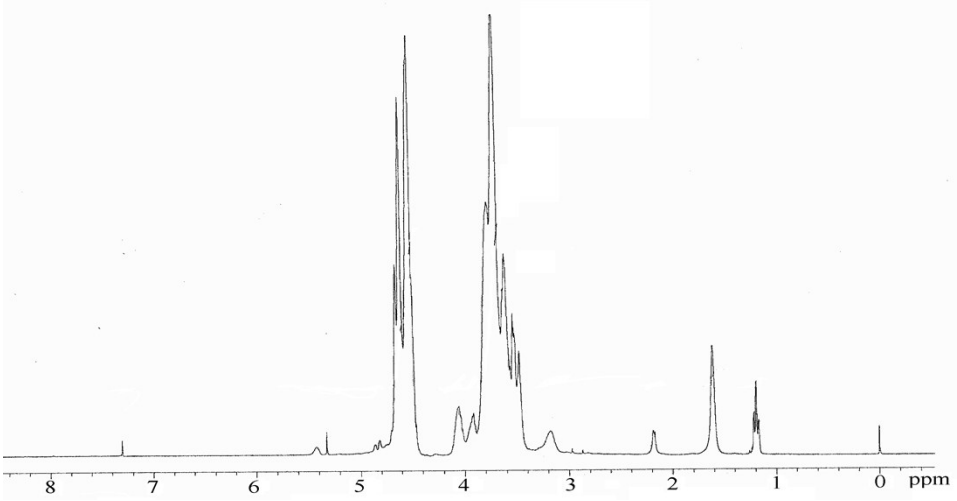


Fig. S6 ^{1}H NMR Spectrum of PGN

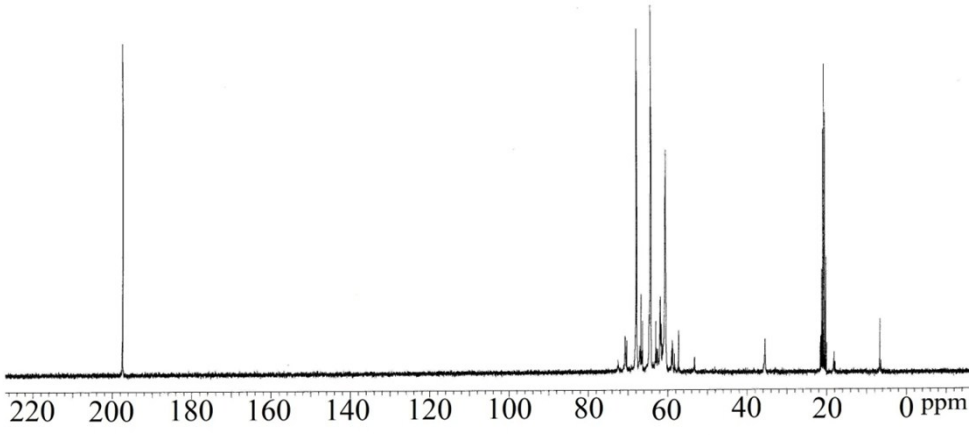
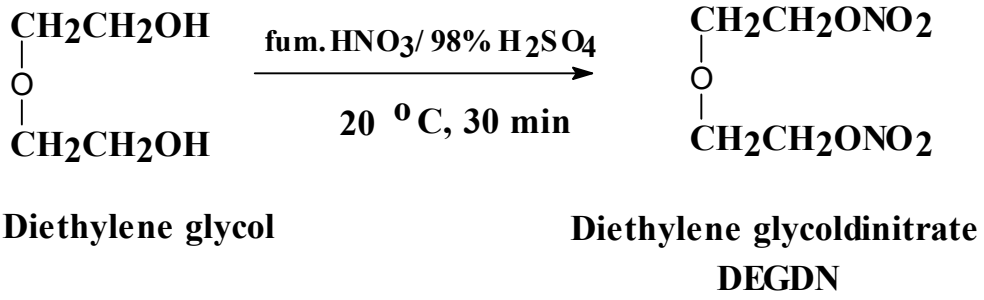


Fig. S7 ^{13}C NMR spectrum of PGN

Synthesis of Diethyleneglycol dinitrate (DEGDN):

The laboratory synthesis of DEGDN was done based on the reported method.[1,2] Fuming HNO_3 (12 ml) and H_2SO_4 (9 ml, 98%) was taken into 3 necked round bottom flask and the reaction mixture was cooled to -5 to 0 ˚C. Diethylene glycol (9 ml, 0.09 moles) was added drop wise to the nitrating mixture (addition time ~30 min) by maintaining the temperature in between -5 to 0 ˚C. Since the reaction is highly exothermic care has to be exercised so that the temperature of the reaction mixture does not go above 0˚C while addition of diethylene glycol. After complete addition, reaction mixture was stirred continuously at 10-15 ˚C for 30 min. Two layers were observed in the reaction mixture (within 7 min).The acid layer was discarded and the organic layer was washed with water several times until pH 6 to 8 and further washed with saturated solution of sodium bicarbonate. The organic layer was dried with anhydrous sodium sulfate to obtain colorless, viscous oily liquid. Yield: (12.95 g, 90%).



Scheme S1. Synthesis of Diethyleneglycol dinitrate (DEGDN)

Characterization:

The FTIR spectrum showed symmetric and asymmetric stretching frequencies at 1278 cm^{-1} and 1633 cm^{-1} due to the presence of -O-NO_2 group. Peaks attributable to C-H and C-O stretching frequencies were observed at 2894 cm^{-1} and 2833 cm^{-1} respectively. C-O-C asymmetric stretching frequency was observed at 1138 cm^{-1} and 2966 cm^{-1} stretching frequency corresponding to C-ONO_2 group (Fig. S8). The ^{1}H-NMR spectrum ($CDCl_3$) showed peaks at 4.6 δ (t, 2H) corresponding to CH_2 attached to O-NO_2 and 3.7 δ (t, 2H) due to the presence of CH_2 attached to oxygen (ether linkage protons C-O-C) (Fig. S9). The ^{13}C NMR spectrum showed the presence of two different peaks at 50.5 and 55.5 due to the presence of C-O-C and C attached to O-NO_2 groups (Fig. S10). The spectroscopic data obtained is in agreement with the reported data in the literature.[1,2]

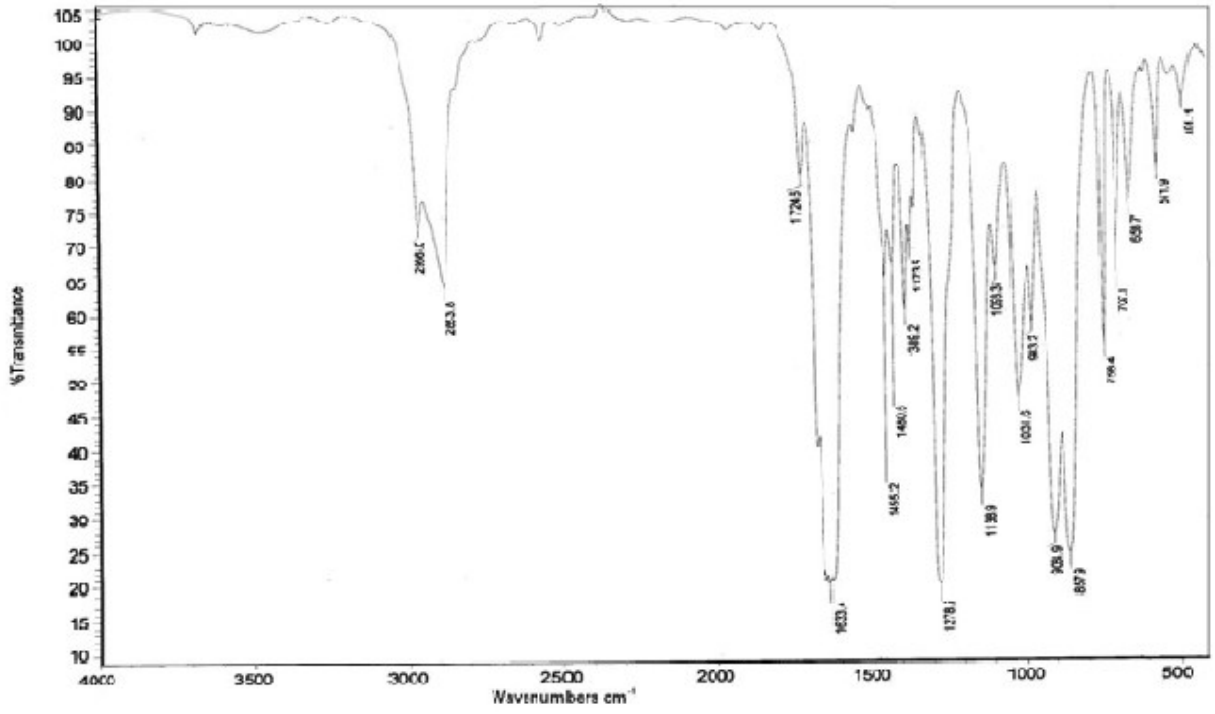


Fig. S8 IR Spectrum of diethyleneglycol dinitrate (DEGDN).

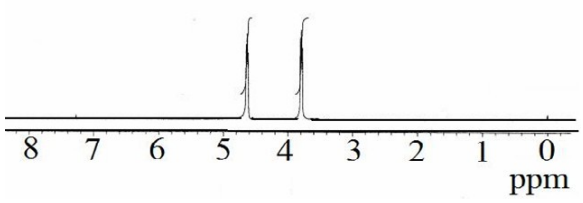


Fig. S9 ^{1}H NMR Spectrum of Diethyleneglycol dinitrate (DEGDN).

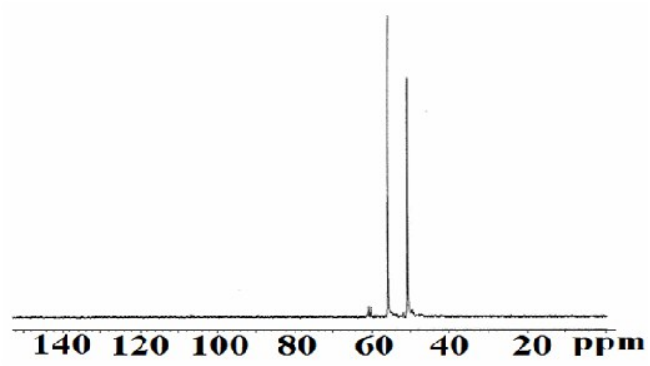


Fig. S10 ^{13}C NMR Spectrum of Diethyleneglycol dinitrate (DEGDN).

Synthesis of N-N-butyl-N`(2-nitroxy-ethyl) nitramine (BuNENA):

BuNENA was synthesised in accordance with the literature method.[3] The synthesis of BuNENA consists of two steps.

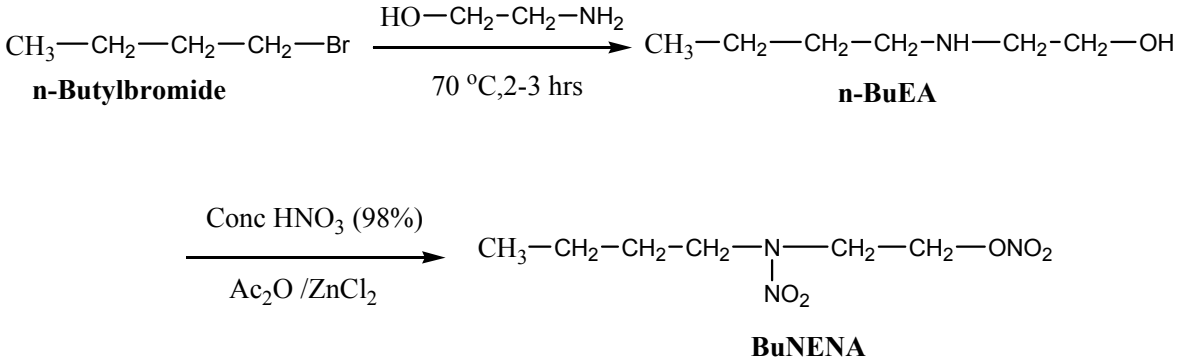
(a) Condensation of n-butyl bromide with ethanol amine

n-Butyl bromide (137g,1 mol) was taken in a three neck round bottom flask. Ethanol amine (61g, 1mol) was added slowly at 70 ˚C. After completion of addition, temperature of the reaction mixture was raised to 120 ˚C and maintained it for 2-3 hours. Then the reaction mixture was cooled to 50 ˚C and poured into 50% NaOH solution. The solution was stirred for some time and the organic layer was separated. On distillation of the organic layer yielded n-Butyl ethanolamine, a colourless viscous liquid. Yield: (100g, 90%),

(b) Nitration of n-Butylethanol amine

Conc. HNO_3 (100 ml, 98%) was taken in a round bottom flask and was cooled in a ice brine bath with agitation to which n-butyl ethanolamine (117g,1 mol) was added at such a rate maintaing the temperature below 22 ˚C. After completion of addition, ice bath was removed and the mixture was stirred at room temperature for 15 to 30 minutes. A solution of acetic anhydride (97%, 240 ml) and Zinc chloride (2.4 g, 17.6 mol) was added maintaining the temperature between 25 ˚C to 30 ˚C. After completion of addition, the mixture is stirred for another one hour. The entire content of the reaction flask was poured in to the crushed ice taken in beaker and stirred for some time. Dense yellow liquid was settled at the bottom of the beaker. The aqueous layer was removed and the organic layer was washed sequentially with distilled water, followed by 5% sodium carbonate and finally with distilled

water. The product was dried with anhydrous sodium sulphate and finally filtered through G-4 crucible under vacuum. Yield: (160 g ,80%)



Scheme S2 Synthesis of N-N-butyl-N`(2-nitroxy-ethyl) nitramine (BuNENA).

Characterization:

The FTIR spectrum of BuNENA (Fig. S11) showed stretching frequencies at 2990 cm^{-1} (C-H str.), 1650 cm^{-1} (s, O-NO_2 str.),1535, 1275 cm^{-1} (s,N-NO_2, asym and sym str.),835 cm^{-1} (b, O-N) respectively.^{1}H NMR (Fig. S12) of BuNENA (300 MHz, $CDCl_3$) δ ppm: 0.96 (t,3H,CH_3), 1.4 (s,2H,CH_2), 1.75 (P,2H,CH_2),3.8 (t,2H,CH_2),4.9 (t,2H,CH_2).

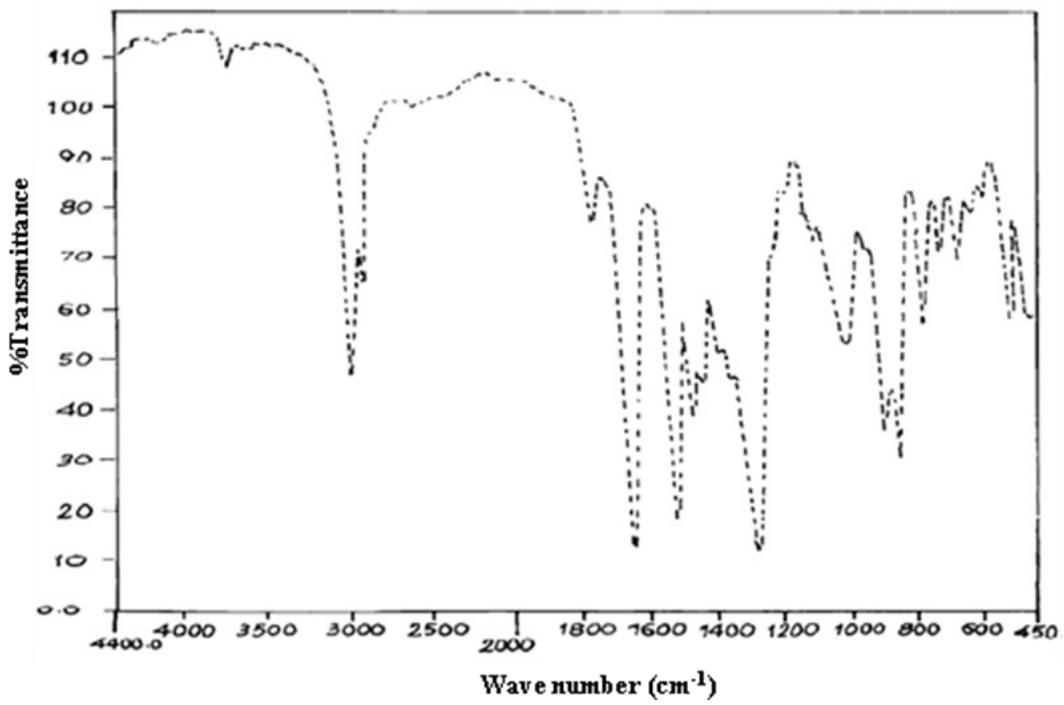


Fig. S11 IR spectrum of N-N-butyl-N`(2-nitroxy-ethyl) nitramine (BuNENA).

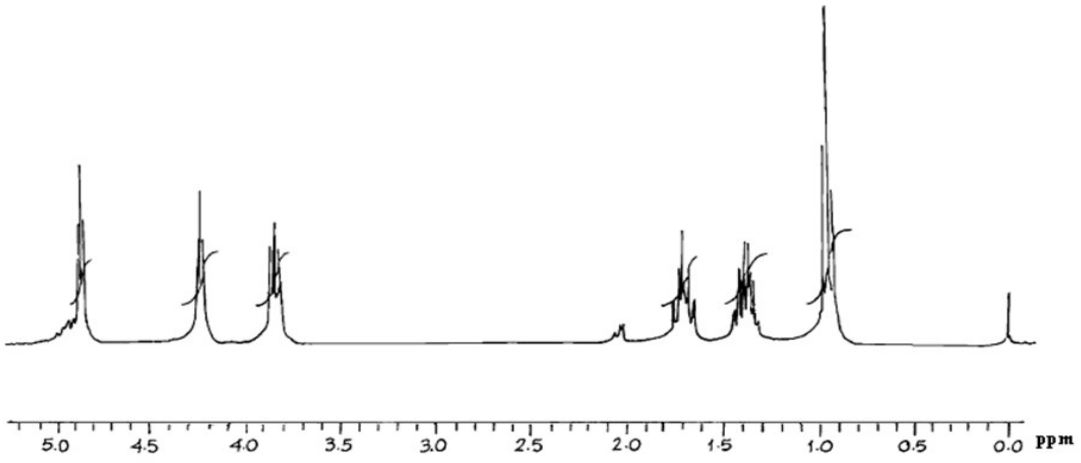


Fig. S12 ^{1}H NMR spectrum of N-N-butyl-N`(2-nitroxy-ethyl) nitramine (BuNENA).

Synthesis of BDNPA:

BDNPA was synthesisized based on the lines of the reported method[4,5] and it involves two steps.

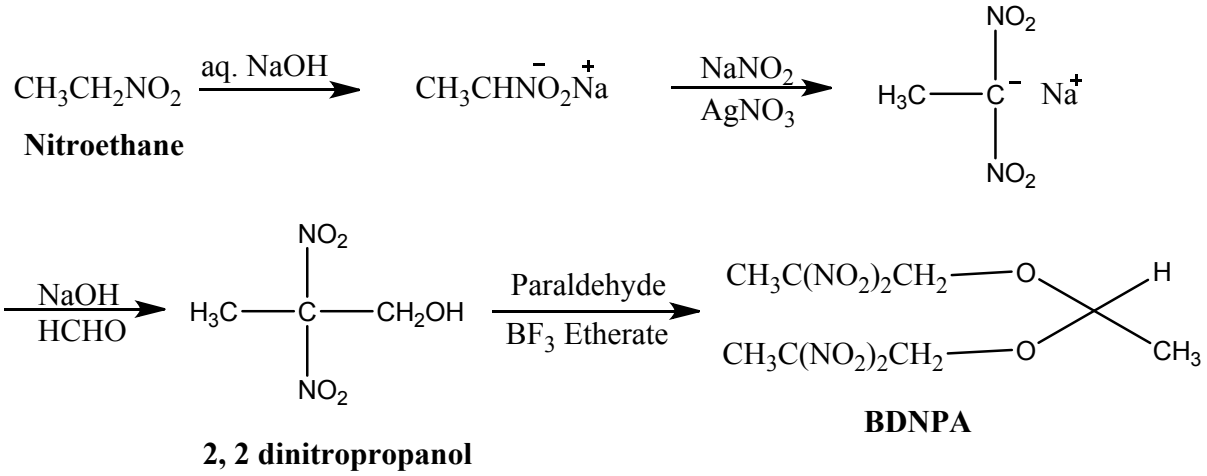
Step-1: Oxidative nitration of nitroethane to form 2, 2 dinitropropanol

Nitroethane (25g, 0.33 mol) was taken into 250 ml three neck round bottom flask equipped with thermowell and addition funnel. The distilled water (68 ml) was added to the above reaction mixture. Then the solution was stirred using magnetic stirrer. Aqueous NaOH solution (60 ml, 50%) was added to this drop wise at 0 to 5˚C within 30 minutes. After complete addition of NaOH solution, sodium nitrite (24g, 0.34 mol) was added all at once and the mixture was stirred for additional 15 minutes. In another 1 lit three neck round bottom flask equipped with addition funnel, thermowell and mechanical stirrer, a solution of $AgNO_3$ (107.8g,0.63 mol in 400 ml distilled water) was cooled to 0 ˚C by using freezing mixture. To this solution, above mixture was added under stirring within 15 to 20 minutes. The temperature increased from 0 to 12-15 ˚C. Stirring continued for additional 30 minutes at temperature of 15-20 ˚C. The pH of the mixture was adjusted to 12-13 by using 110 ml of 50% aq NaOH solution. Stirring continued for 20 to 25 minutes. The mixture was filtered on Buchner funnel. Then it was washed four times with 55 ml of distilled water. Filtrate and washings were collected into filtration flask. The solution was stirred using magnetic stirrer and pH was adjusted using glacial acetic acid to 8.5-9.5. To this solution 37% of formaldehyde (44 ml) was added all at once and pH is further adjusted to 5 using acetic acid over 30 minutes period. The solution was stirred for one hour and then

was extracted four times with 125 ml of dichloromethane and dried over sodium sulphate. The dichloromethane was removed by using rotary evaporator. Yield: (40g, 80%)

Step-2: Synthesis of Bis(2,2 dinitropropyl)acetal

In a 500 ml four neck round bottom flask equipped with mechanical stirrer, mercury seal, addition funnel, thermowell and guard tube. Dinitropropanol (80g, 0.53 mol), paraldehyde (24 ml) and dichloromethane (240 ml) were added and cooled to -8 to -10 ˚C using freezing mixture. BF_3 etherate (48 ml) was added drop wise to this solution under stirring, maintaining the temperature between -8 to -10 ˚C. Stirring continued for 1 hour at -8 to -10 ˚C and then the contents were poured into ice water mixture and stirred for 10 minutes. Organic layer was separated and washed with 5% aq NaOH solution two times using 100 ml aliquot at a time and then with 100 ml of distilled water. Organic layer dried on sodium sulphate and the solvent was removed using rotary evaporator. Yield: (77g, 60 %).



Scheme S3 Synthesis of bis(2,2-dinitropropyl)acetal (BDNPA).

Characterization:

The IR spectrum (Fig. S13) of BDNPA shows the characteristic peaks of gem-diniro group frequencies at 1576 cm^{-1}(assymetric,-C-NO_2 str.), 1328 cm^{-1} (symmetric, -C-NO_2 str.), 1142, 1018 cm^{-1} (s,-C-O-C- str.).^{1}H NMR (Fig. S14) of BDNPA (90 MHz, $CDCl_3$) δ ppm: 2.1 δ (6H singlet), 1.3 δ (3H doublet), 4.2 δ (4H singlet), 4.8 δ (1H quarterlet). The data obtained in the current study enriches the existing scientific data of this material.

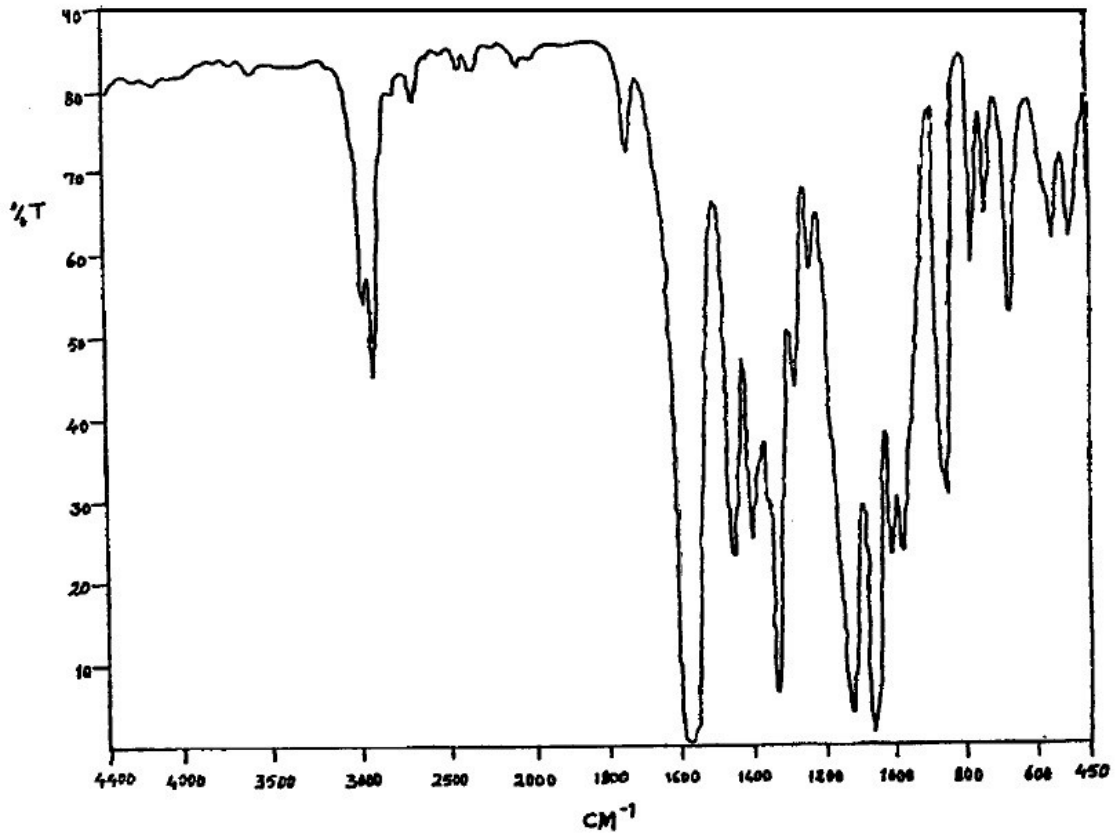


Fig. S13 IR spectrum of bis(2,2-dinitropropyl)acetal (BDNPA).

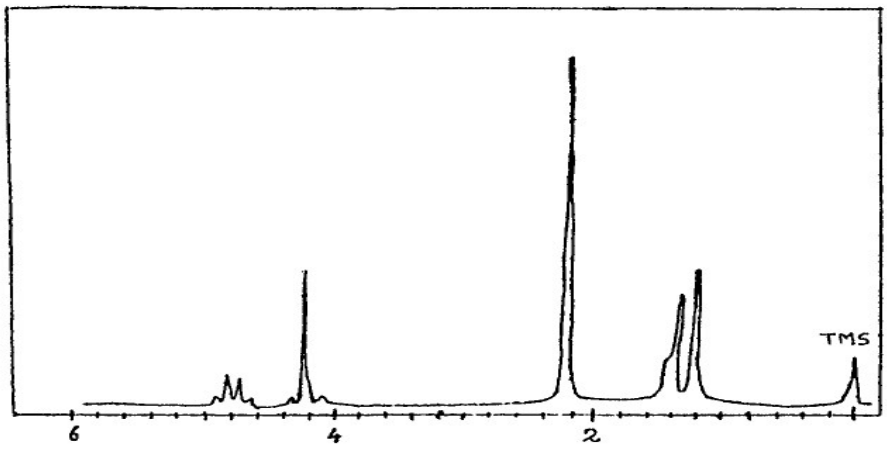


Fig. S14 ^{1}H NMR spectrum of bis(2,2-dinitropropyl)acetal (BDNPA).

The other two plasticizers viz. 1,2,4-butanetriol trinitrate (BTTN) and Dinitro-diaza-alkanes (DNDA-57) were supplied by the trades viz. Bharat Explosives Ltd. Lalitpur, India and Indian

Adhesives & Glues, Pune, India, respectively and used as such without further purification and characterization.

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