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Supplementary Information

A Molecular Dynamics Study of Plasticiser Migration in Nitrocellulose Binders

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Construction of Simulation Cells

ethyl centralite (EC)

Unit cell dimensions (monoclinic), a = 9.6990 Å, b = 16.7622 Å, c = 10.6011 Å
Z = 4 per unit cell
Cubic symmetry assumed, unit cell dimensions used to calculate volume
9.70 Å × 16.76 Å × 10.60 Å = 1723 Å^3
40 Å × 40 Å × 40 Å = 64,000 Å^3
64,000 Å^3 / 1723 Å^3 = 37.14
37.14 × 4 ~ **149** ethyl centralite molecules in 40 Å^3

1-nitramino-2,3-dinitroxypropane (NG-N1)

unit cell dimensions (monoclinic), a = 7.1363 Å, b = 8.6355 Å, c = 13.7048 Å
Z = 4 per unit cell
Cubic symmetry assumed, unit cell dimensions used to calculate volume
7.1 Å × 8.6 Å × 13.7 Å = 837 Å^3
40 Å × 40 Å × 40 Å = 64,000 Å^3
64,000 Å^3 / 837 Å^3 = 76.46
76.46 × 4 = ~ **306** NG-N1 molecules in 40 Å^3

NC, NG-N1 and 2,4-DNEB binder system

NC model = 40 dimers
Mass of one dimer = 594
Mass of 1 NC model = 23,760

NC : plasticizer = 1 : 8 ratio [1]

23,760 × 8 = 190,080
Mass of plasticizer = 190,080

% mass of plasticizer that NG-N1 = 34%
190,080 × 0.34 = 64,627 ÷ NG-N1 Mr 226
= **286** NG-N1 molecules

% mass of plasticizer that 2,4-DNEB = 66%
190,080 × 0.66 = 125,453 ÷ 2,4-DNEB Mr 196
= **640** 2,4-DNEB molecules

NC, 2,4-DNEB and 2,4,6-TNEB binder system

NC model = 40 dimers
Mass of one dimer = 594
Mass of 1 NC model = 23,760

NC : plasticizer = 1 : 8 ratio [1]

23,760 × 8 = 190,080
Mass of plasticizer = 190,080

% mass of plasticizer that is 2,4,6-TNEB = 35%
190,080 × 0.35 = 66,528 ÷ 2,4,6-TNEB Mr 241
= **276** 2,4,6-TNEB molecules

% mass of plasticizer that 2,4-DNEB = 65%
190,080 × 0.65 = 123,552 ÷ 2,4-DNEB Mr 196
= **630** 2,4-DNEB molecules

Total mass of ingredients for both binder systems = 213,840 (23,760 + 190,080)
1% 213,840 = 2138 ÷ EC Mr 268
= **8** EC molecules

(1) Willcox, M.; Padfield, J.; McAteer, D. *Demonstration of 1-Nitramino-2,3-Dinitroxypropane as an Energetic Plasticiser Component in an HMX-Based PBX*; Shrivenham.

NC Force-Field Parameters

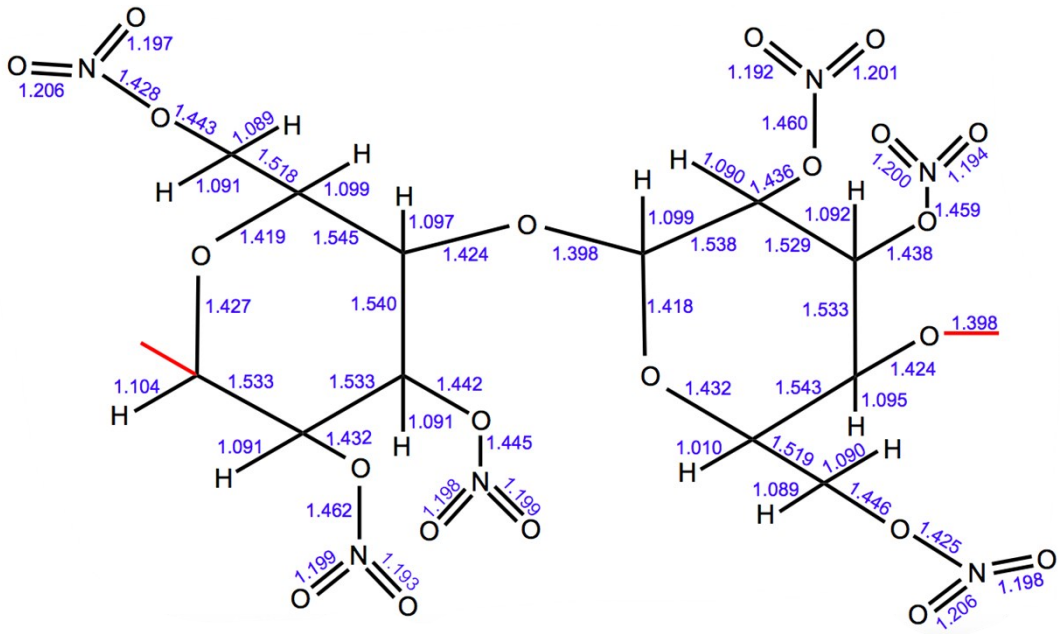

Figure S1 – The QM bond lengths for NC

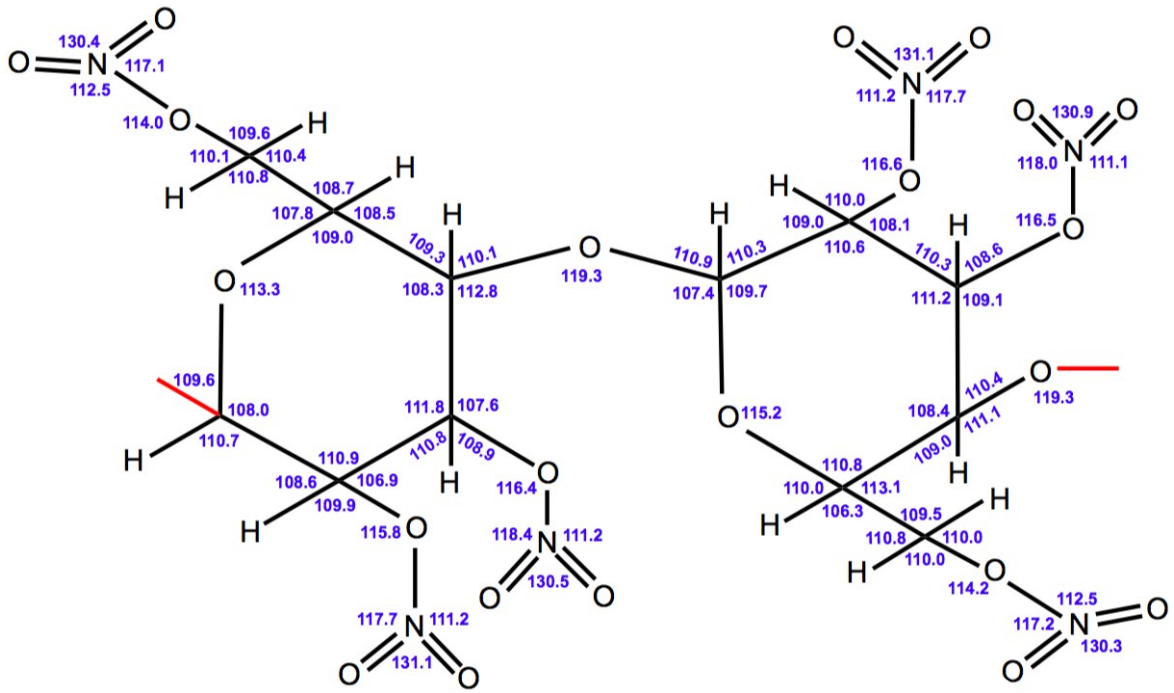

Figure S2 – The QM bond angles for NC

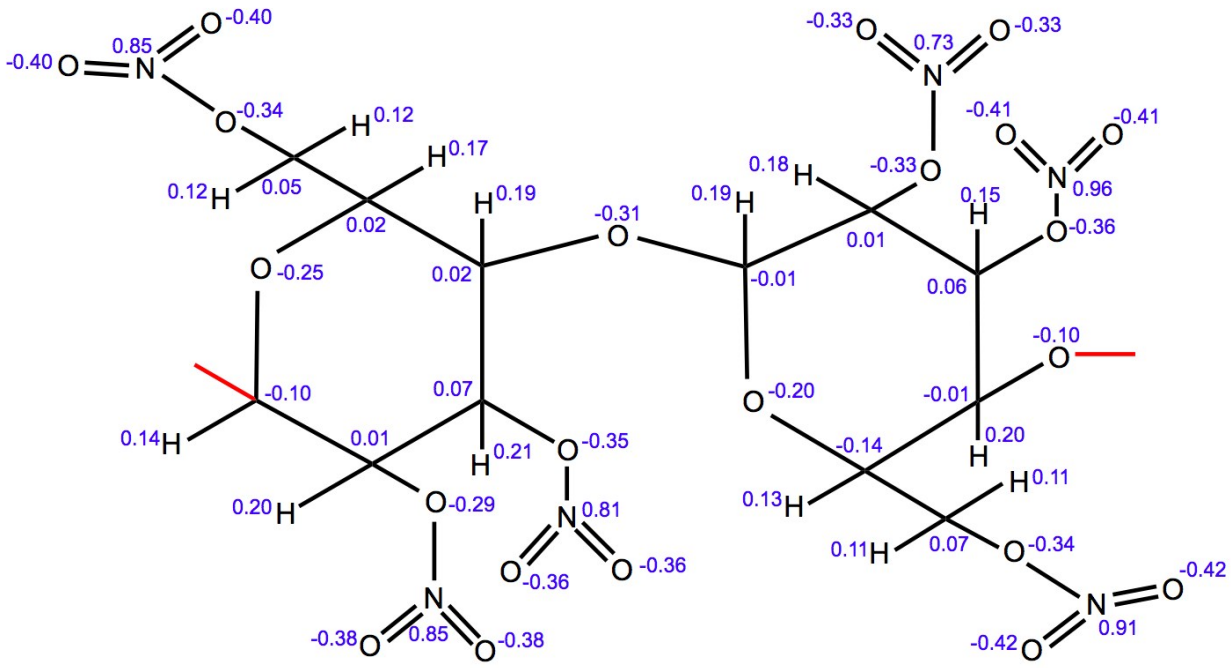

Figure S3 – The QM derived partial charges for NC

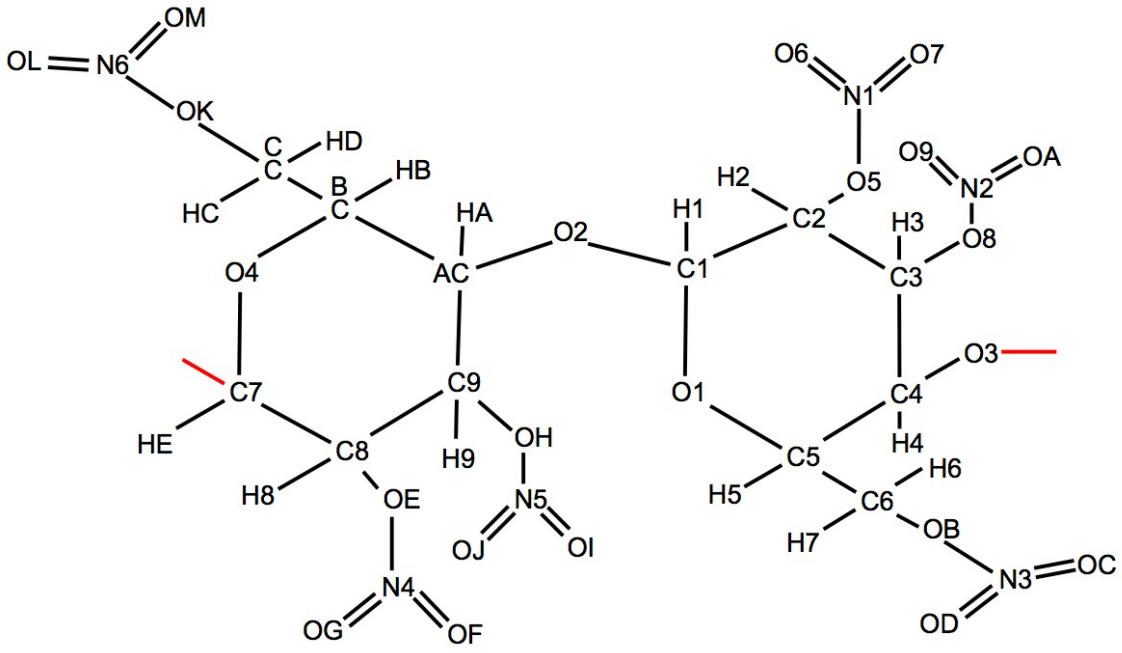

Figure S4 – Atom types for NC

Table S1 - Bond angles and their associated force constants for NC

angle label	angle (°)	angle force constant kcal mol^{-1}	angle label	angle (°)	angle force constant kcal mol^{-1}
C1-O2-CA	119.3	40.737	C7-O3-C4	119.3	40.737
C1-O1-C5	115.2	33.674	C7-O4-CB	113.3	43.073
C1-C2-O5	108.0	43.798	C7-C8-C9	110.9	53.836
C1-C2-H2	109.0	41.389	C7-C8-H8	108.6	90.739
C1-C2-C3	110.6	48.275	C7-C8-OE	110.1	44.254
C2-O5-N1	116.6	39.885	C8-OE-N4	115.8	46.435
C2-C3-O8	108.3	34.442	C8-C9-H9	110.8	20.996
C2-C3-H3	110.3	28.754	C8-C9-CA	111.8	55.362
C2-C3-C4	111.2	36.517	C8-C9-OH	108.4	26.239
C3-O8-N2	116.5	47.412	C8-C7-HE	110.7	27.117
C3-C4-H4	109.6	56.511	C8-C7-O4	108.0	80.084
C3-C4-O3	110.4	43.839	C9-OH-N5	116.4	47.485
C3-C4-C5	108.4	43.745	C9-CA-CB	108.3	65.648
C3-C2-O5	108.1	43.652	C9-CA-HA	109.4	50.893
C3-C2-H2	111.3	25.682	CA-CB-CC	112.3	38.759
C4-O3-C7	119.3	40.737	CA-CB-HB	108.5	25.395
C4-C5-H5	108.5	30.250	CA-CB-O4	109.0	37.218
C4-C5-C6	113.1	36.787	CA-C9-H9	109.4	60.609
C4-C5-O1	110.8	43.606	CB-CC-OK	105.2	34.184
C4-C3-O8	109.1	23.300	CB-CC-HC	110.8	40.967
C4-C3-H3	109.3	26.885	CB-CC-HD	110.4	37.992
C5-C6-OB	106.8	55.967	O4-CB-CC	107.8	40.649
C5-C6-H6	109.5	65.325	O4-CB-HB	110.6	25.209
C5-C6-H7	110.8	15.878	O4-C7-HE	108.9	20.175
C5-C4-H4	109.0	42.677	O3-C7-HE	111.4	21.864
C5-C4-O3	108.3	37.763	O3-C7-O4	109.6	46.948
O1-C5-H5	110.0	21.832	O3-C4-C5	108.3	37.763
O1-C5-C6	108.2	42.454	CC-OK-N6	114.0	44.111
O1-C1-C2	109.7	44.416	O5-N1-O7	117.7	34.744
O1-C1-O2	107.4	46.583	O5-N1-O6	111.2	34.048
O1-C1-H1	110.2	39.545	O6-N1-O7	131.1	29.981
O2-CA-CB	106.9	40.242	O8-N2-OA	111.1	44.660
O2-CA-HA	110.1	29.973	O8-N2-O9	118.0	34.056
O2-CA-C9	112.8	53.169	O9-N2-OA	130.9	36.758
O2-C1-C2	108.3	48.945	OB-N3-OC	112.5	37.951
O3-C7-C8	108.2	47.206	OB-N3-OD	117.2	36.769
O3-C4-H4	111.1	21.617	OD-N3-OC	130.3	35.003
C6-OB-N3	114.2	39.895	OE-N4-OG	117.7	47.453
C6-C5-H5	106.3	30.776	OE-N4-OF	111.2	53.902
OE-C8-C9	106.9	36.954	H1-C1-O2	110.9	16.912
OE-C8-H8	109.9	87.142	H2-C2-O5	110.0	48.895
OF-N4-OG	131.1	69.151	H3-C3-O8	108.6	34.106
OH-N5-OI	111.2	55.446	H6-C6-OB	110.0	27.343
OH-N5-OJ	118.4	52.591	H7-C6-OB	110.0	24.304
OH-C9-H9	108.9	46.239	H7-C6-H6	109.7	31.314
OH-C9-CA	107.6	45.535	H8-C8-C9	110.5	55.266
OJ-N5-OI	130.5	82.862	HA-CA-CB	109.3	50.527
OK-N6-OM	117.1	57.325	HB-CB-CC	108.7	19.454
OK-N6-OL	112.5	57.329	HC-CC-OK	110.1	41.757
OL-N6-OM	130.4	101.28	HD-CC-OK	109.6	39.516
H1-C1-C2	110.3	50.458	HD-CC-HC	110.6	16.169

Table S2 - Bond lengths and their associated force constants for NC

bond label	bond length (Å)	bond force constant kcal mol^{-1}	bond label	bond length (Å)	bond force constant kcal mol^{-1}
C1-O1	1.418	239.053	CC-OK	1.443	215.298
C1-H1	1.099	76.391	N1-O6	1.192	606.817
C1-O2	1.398	202.201	N1-O7	1.201	569.798
C1-C2	1.538	73.590	O8-N2	1.459	41.589
C2-C3	1.529	173.643	N2-O9	1.200	513.678
C2-H2	1.090	492.373	N2-OA	1.194	134.523
C2-O5	1.436	184.887	OB-N3	1.425	86.445
C3-C4	1.533	207.598	N3-OD	1.206	547.654
C3-H3	1.092	326.109	N3-OC	1.198	589.928
C3-O8	1.438	189.688	OE-N4	1.462	25.921
C4-C5	1.543	178.092	N4-OF	1.193	518.846
C4-O3	1.424	216.279	N4-OG	1.199	454.922
C4-H4	1.095	153.217	OH-N5	1.445	51.727
C5-O1	1.432	174.002	N5-OJ	1.198	506.022
C5-C6	1.519	211.477	N5-OI	1.199	204.762
C5-H5	1.010	313.828	OK-N6	1.428	132.208
O2-CA	1.424	216.279	N6-OL	1.197	219.723
O3-C7	1.398	216.279	N6-OM	1.206	165.962
C6-H7	1.089	314.277	O5-N1	1.460	103.967
C6-H6	1.090	264.806	C8-C9	1.533	177.711
C6-OB	1.446	226.092	C9-OH	1.442	176.667
C7-O3	1.398	202.201	C9-CA	1.540	166.559
C7-C8	1.533	106.275	C9-H9	1.091	147.034
C7-O4	1.427	278.244	CA-HA	1.097	270.248
C7-HE	1.104	282.007	CA-CB	1.545	97.561
C8-OE	1.432	193.333	CB-O4	1.419	244.525
C8-H8	1.091	336.078	CB-HB	1.099	294.432
			CB-CC	1.518	198.880
			CC-HD	1.089	295.255
			CC-HC	1.091	303.253

Table S3 - Dihedral angles for NC

Dihedral Angle	Number of paths [a]	V_n [b]	γ [c]	n [d]
C – O – C – C	3	1.150	0.000	3.000
C – O – C – H	3	1.150	0.000	3.000
C – C – C – C	1	0.200	180.0	1.000
C – C – C – H	1	0.160	0.000	3.000
C – C – C – O	9	1.400	0.000	3.000
C – C – O – N	3	1.150	0.000	3.000
C – O – N – O	1	1.100	180.0	2.000
C – O – C – O	9	1.400	0.000	3.000
O – C – C – O	1	1.175	0.000	2.000
O – C – C – H	1	0.250	0.000	1.000
N – O – C – H	3	1.150	0.000	3.000
H – C – C – H	0	0.150	0.000	3.000

a – number of bond paths that total V_n must be divided by, b – magnitude of the torsion in kcal mol^{-1}, c – phase angle in degrees, d – periodicity of the torsion

Table S4 - Initial Lennard-Jones parameters for NC

Atom	R_{min} [a]	ε [b]
C	1.9080	0.1094
O_{ether}	1.6837	0.1700
N	1.8240	0.1700
$O_{nitro\ grp.}$	1.6612	0.2100
H	1.4870	0.0157

a - the distance where the potential reaches a minimum in Angstroms ($\sigma \times 2^{1/6}$), b - the potential well depth in kcal mol^{-1}

NG-N1 Force-Field Parameters

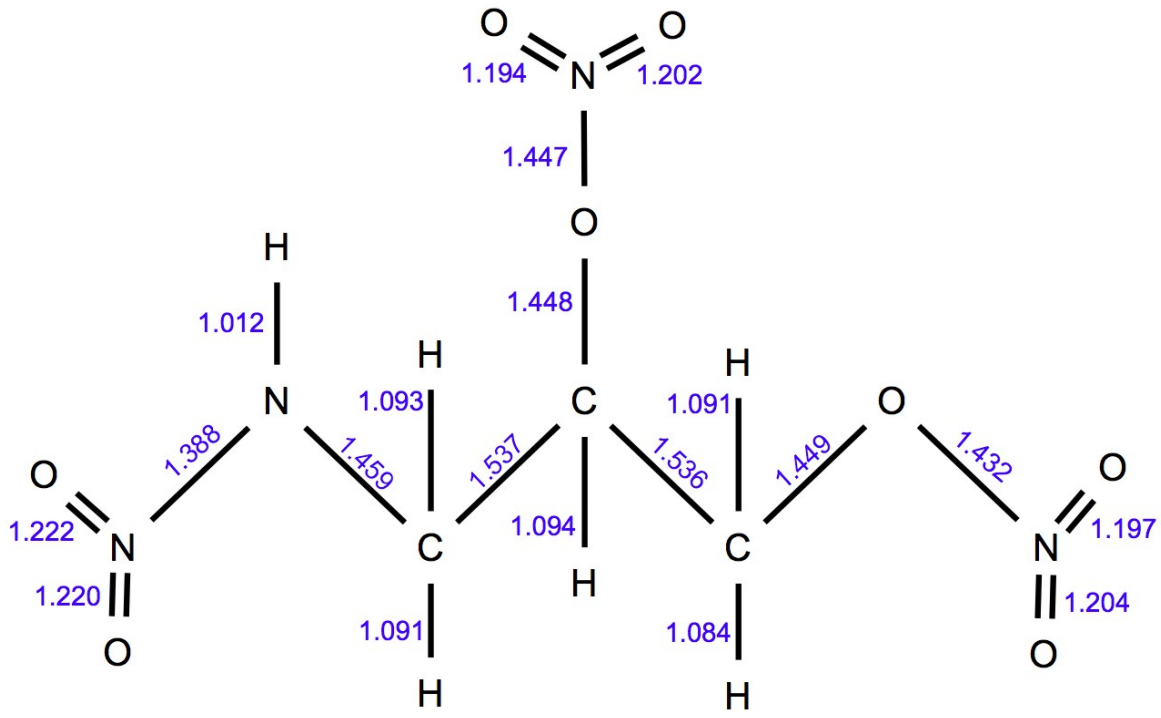

Figure S5 – The QM bond lengths for NG-N1

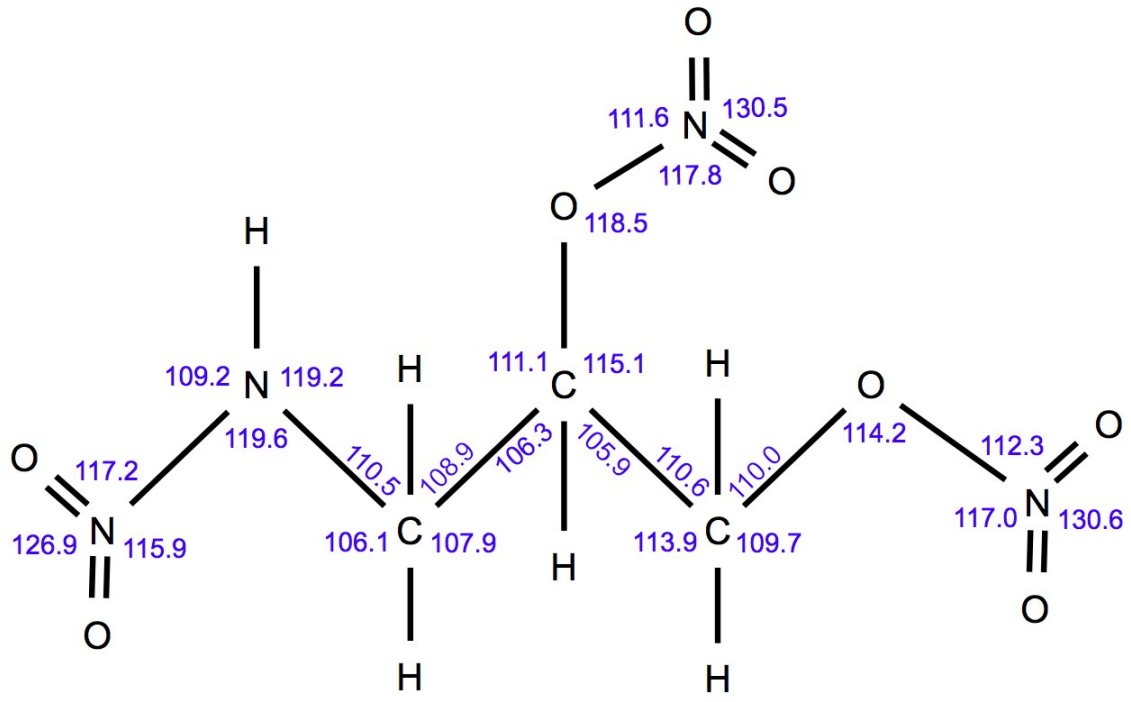

Figure S6 – The QM bond angles for NG-N1

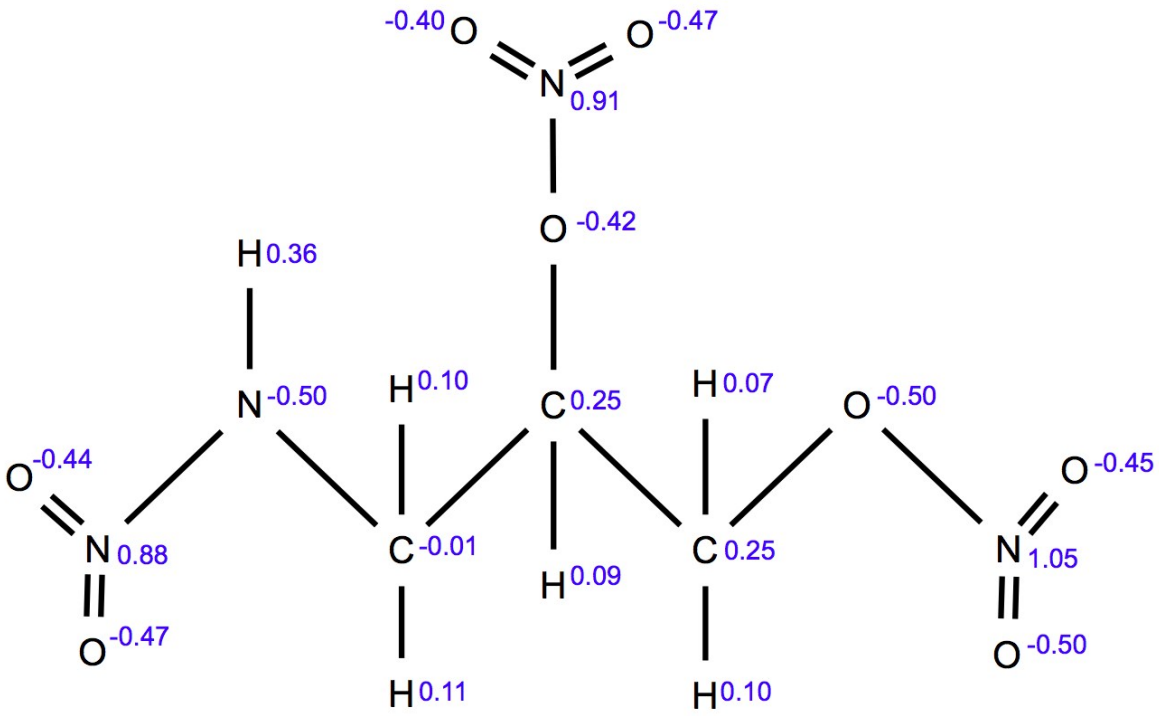

Figure S7 – The QM derived partial charges for NG-N1

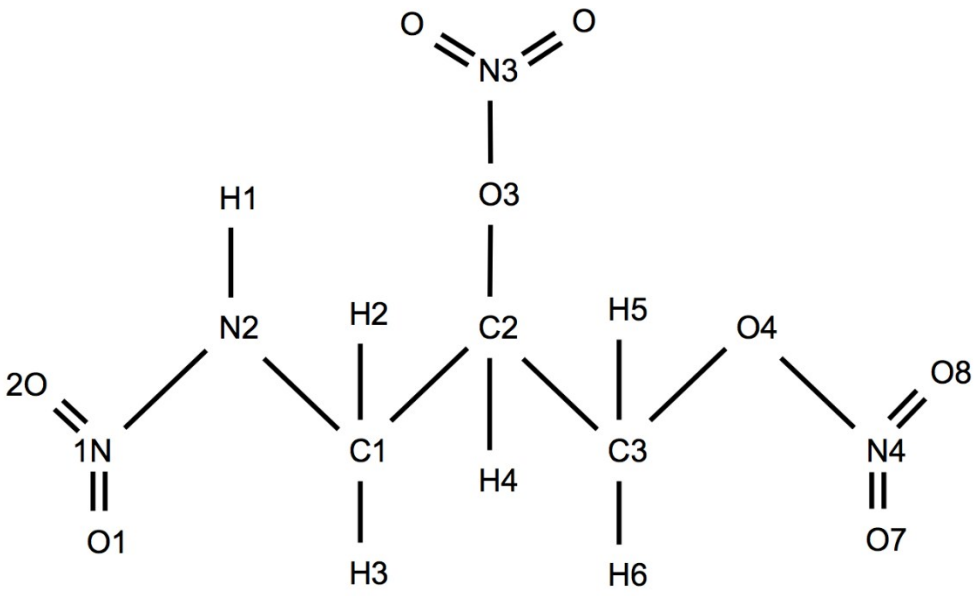

Figure S8 - Atom types for NG-N1

Table S5 - Bond angles and their associated force constants for NG-N1

angle label	angle (°)	angle force constant kcal mol^{-1}	angle label	angle (°)	angle force constant kcal mol^{-1}
N1-N2-H1	109.2	44.456	C2-C3-H5	110.6	40.805
N1-N2-C1	119.6	53.399	C2-C3-H6	113.9	35.379
O1-N1-O2	126.9	32.668	C2-O3-N3	114.2	36.206
O1-N1-N2	115.9	45.328	C3-C2-O3	115.1	38.968
O2-N1-N2	117.2	49.030	C3-C2-H4	105.9	20.409
N2-C1-H2	110.5	21.422	C3-O4-N4	114.2	36.206
N2-C1-H3	106.1	45.849	O3-C2-H4	99.80	42.500
N2-C1-C2	115.1	43.126	O3-N3-O5	117.0	45.368
H1-N2-C1	119.2	16.728	O3-N3-O6	112.3	40.518
H2-C1-H3	108.4	17.335	O4-C3-H5	110.0	27.784
H2-C1-C2	108.9	17.579	O4-C3-H6	109.7	40.766
H3-C1-C2	107.9	39.138	O4-N4-O7	117.0	45.368
C1-C2-C3	116.6	45.130	O4-N4-O8	112.3	40.518
C1-C2-O3	111.1	32.356	O5-N3-O6	130.5	67.287
C1-C2-H4	106.3	45.519	O7-N4-O8	130.6	58.512
C2-C3-O4	101.9	60.140	H5-C3-H6	110.4	42.5

Table S6 - Bond lengths and their associated force constants for NG-N1

bond label	bond length (Å)	bond force constant kcal mol^{-1}	bond label	bond length (Å)	bond force constant kcal mol^{-1}
N1-O1	1.220	530.96	C2-H4	1.094	88.641
N1-O2	1.222	515.10	C3-O4	1.449	144.48
N1-N2	1.388	163.58	C3-H5	1.091	262.88
N2-H1	1.012	353.36	C3-H6	1.084	241.61
N2-C1	1.459	243.44	O4-N4	1.432	115.55
H2-C1	1.093	320.79	O3-N3	1.472	115.55
H3-C1	1.091	101.87	N3-O5	1.202	590.69
C1-C2	1.537	249.54	N3-O6	1.194	383.69
C2-C3	1.536	185.49	N4-O7	1.204	568.39
C2-O3	1.448	170.08	N4-O8	1.197	598.04

Table S7 - Dihedral angles for NG-N1

Dihedral Angle	Number of paths [a]	V_n [b]	γ [c]	n [d]
$C - C - C - O_{ether}$	1	0.300	180.0	2.000
$N_{amine} - C - C - O_{ether}$	1	0.300	180.0	2.000
$H - C - C - H$	1	0.300	180.0	2.000
$N_{nitro} - N_{amine} - C - H$	1	2.500	180.0	2.000
$N_{nitro} - N_{amine} - C - C$	1	2.500	180.0	2.000
$O_{nitro} - N_{amine} - N_{nitro} - H$	1	1.150	000.0	2.000
$O_{nitro} - N_{amine} - N_{nitro} - C$	1	1.150	000.0	2.000
$N_{amine} - C - C - C$	1	0.300	180.0	2.000
$N_{amine} - C - C - H$	1	0.300	180.0	2.000
$H - N_{amine} - C - H$	1	2.500	180.0	2.000
$H - N_{amine} - C - C$	1	2.500	180.0	2.000
$H - C - C - C$	1	0.300	180.0	2.000
$H - C - C - O_{ether}$	1	0.300	180.0	2.000
$C - C - O_{ether} - N_{nitro}$	3	1.150	000.0	3.000
$C - O_{ether} - N_{nitro} - O_{nitro}$	2	6.000	180.0	2.000
$O_{ether} - C - C - O_{ether}$	1	0.300	180.0	2.000
$N_{nitro} - O_{ether} - C - H$	3	1.150	000.0	3.000

a – number of bond paths that total V_n must be divided by, b – magnitude of the torsion in kcal mol^{-1}, c – phase angle in degrees, d – periodicity of the torsion

Table S8 - Initial Lennard-Jones parameters for NG-N1

Atom	R_{min} [a]	ε [b]
N_{nitro}	1.8240	0.1200
N_{amine}	1.8240	0.1700
O_{nitro}	1.6612	0.2100
O_{ether}	1.6837	0.1700
C	1.9080	0.1094
H_{amine}	0.6000	0.0157
H	1.4870	0.0157

a - the distance where the potential reaches a minimum in Angstroms ($\sigma \times 2^{1/6}$), b - the potential well depth in kcal mol^{-1}

EC Force-Field Parameters

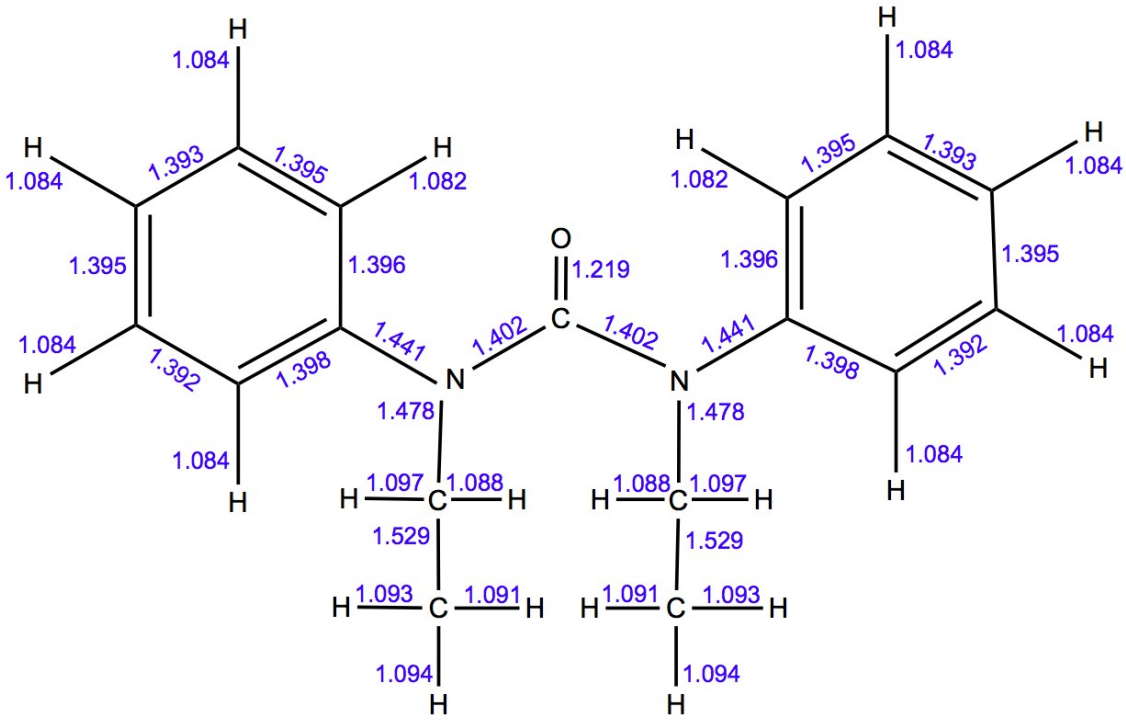

Figure S9 – The QM bond lengths for EC

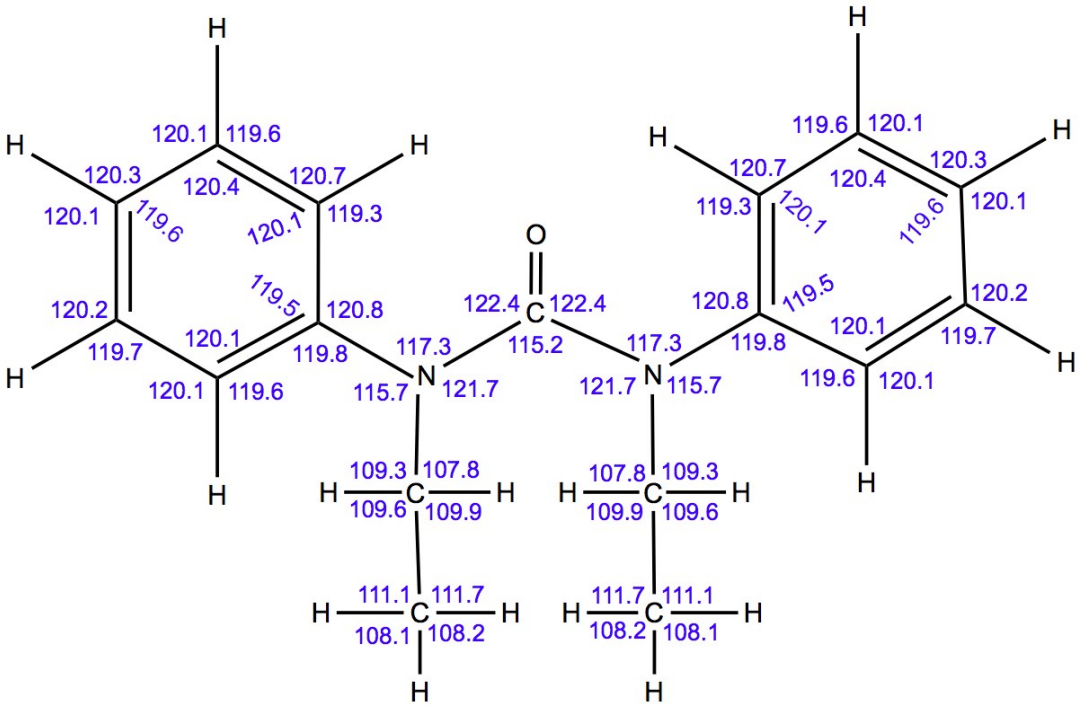

Figure S10 – The QM bond angles for EC

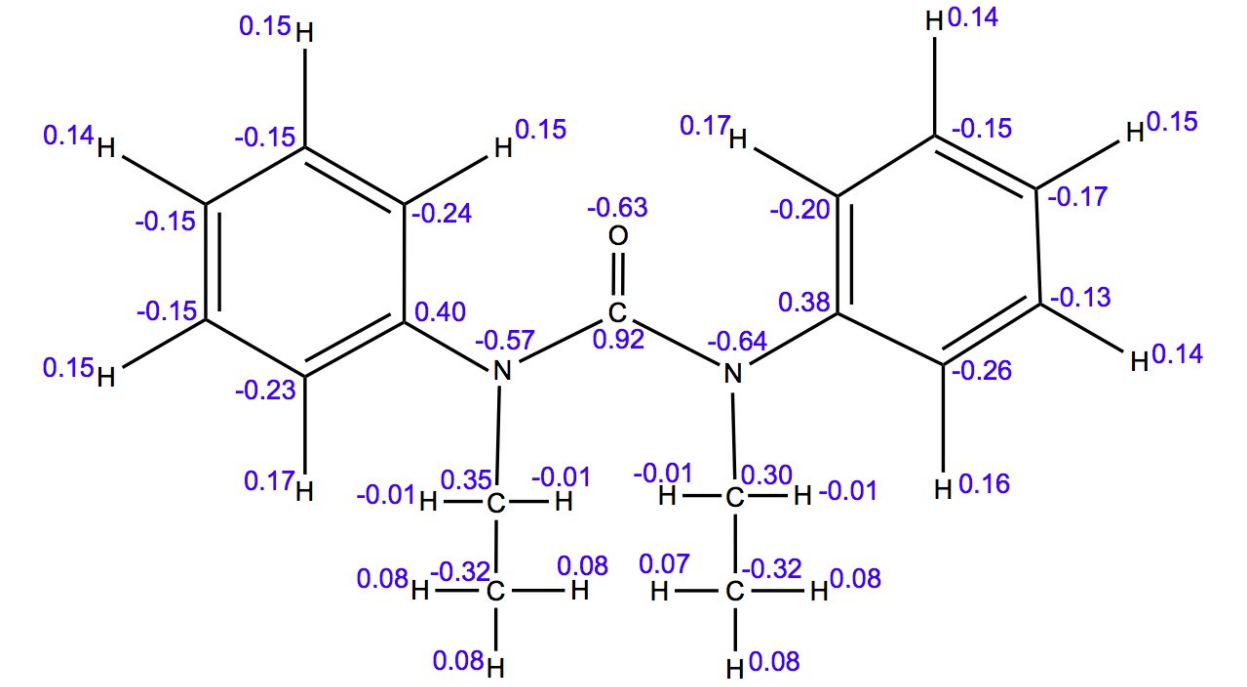

Figure S11 – The QM derived partial charges for EC

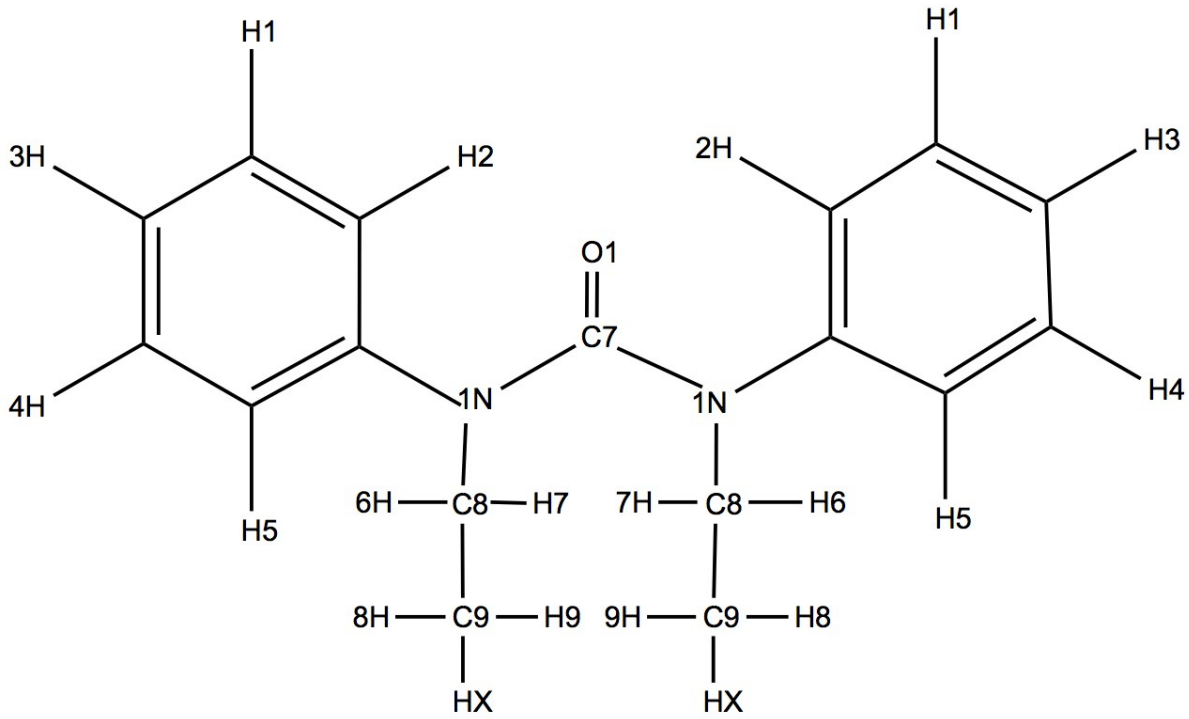

Figure S12 - Atom types for EC

Table S9 - Bond angles and their associated force constants for EC

angle label	angle (°)	angle force constant kcal mol^{-1}	angle label	angle (°)	angle force constant kcal mol^{-1}
C4-C6-C5	120.1	50.753	C3-C4-H4	120.2	9.196
C4-C6-H5	120.1	27.276	C3-C1-H1	120.1	28.583
C4-C3-C1	119.6	53.963	N1-C7-N1	115.2	37.543
C4-C3-H3	120.1	43.327	N1-C7-O1	122.4	41.923
C6-C4-C3	120.1	67.422	N1-C8-C9	113.2	49.143
C6-C4-H4	119.7	38.032	N1-C8-H7	107.8	27.705
C6-C5-C2	119.5	74.000	N1-C8-H6	109.3	41.157
C6-C5-N1	119.8	56.555	C7-N1-C8	121.7	39.851
C5-C6-H5	119.6	28.835	C8-C9-H8	111.1	49.577
C5-C2-C1	120.1	54.231	C8-C9-HX	109.7	20.654
C5-C2-H2	119.3	35.361	C8-C9-H9	111.7	32.833
C5-N1-C7	117.3	37.401	C9-C8-H7	109.9	29.740
C5-N1-C8	115.7	36.180	C9-C8-H6	109.6	45.166
C2-C5-N1	120.8	63.310	H7-C8-H6	107.0	18.086
C2-C1-C3	120.4	51.354	HX-C9-H9	108.2	14.231
C2-C1-H1	119.6	27.167	HX-C9-H8	108.1	22.147
C1-C2-H2	120.7	39.197	H9-C9-H8	108.1	30.004
C1-C3-H3	120.3	42.653			

Table S10 - Bond lengths and their associated force constants for EC

bond label	bond length (Å)	bond force constant kcal mol^{-1}	bond label	bond length (Å)	bond force constant kcal mol^{-1}
C4-C6	1.392	280.76	C3-H3	1.084	256.40
C4-C3	1.395	211.40	N1-C7	1.402	227.41
C4-H4	1.084	187.89	N1-C8	1.478	160.70
C6-C5	1.398	280.14	C7-O1	1.219	654.10
C6-H5	1.084	112.12	C8-C9	1.529	171.52
C5-C2	1.396	248.10	C8-H7	1.088	307.06
C5-N1	1.441	229.62	C8-H6	1.097	160.82
C2-C1	1.395	278.56	C9-H8	1.093	234.00
C2-H2	1.082	173.56	C9-H9	1.091	225.00
C1-C3	1.393	334.20	C9-HX	1.094	308.57
C1-H1	1.084	125.97	C9-H9	1.093	288.02

Table S11 - Dihedral angles for EC

Dihedral Angle	Number of paths [a]	V_n [b]	γ [c]	n [d]
$C_{ar} - C_{ar} - C_{ar} - C_{ar}$	1	14.50	180.0	2.000
$C_{ar} - C_{ar} - C_{ar} - N$	1	14.50	180.0	2.000
$C_{ar} - C_{ar} - C_{ar} - H$	1	1.100	180.0	2.000
$C_{ar} - C_{ar} - N - C_{carbonyl}$	4	1.800	180.0	2.000
$C_{ar} - C_{ar} - N - C_{al}$	4	1.800	180.0	2.000
C – N – C – N	4	10.00	180.0	2.000
C – N – C – O	4	10.00	180.0	2.000
$C_{ar} - N - C_{al} - C_{al}$	6	1.800	0.000	3.000
$C_{ar} - N - C_{al} - H$	6	1.800	0.000	3.000
$H - C_{ar} - C_{ar} - H$	1	1.100	180.0	2.000
$H - C_{ar} - C_{ar} - N$	1	14.50	180.0	2.000
$H - C_{al} - C_{al} - N$	1	0.300	180.0	2.000
$C_{carbonyl} - N - C_{al} - C_{al}$	6	1.800	0.000	3.000
$C_{carbonyl} - N - C_{al} - H$	6	1.800	0.000	3.000
$H - C_{al} - C_{al} - H$	1	0.300	180.0	2.000

a – number of bond paths that total V_n must be divided by, b – magnitude of the torsion in kcal mol^{-1}, c – phase angle in degrees, d – periodicity of the torsion, ar – aromatic, al – aliphatic

EC Force-Field Non-Bonding Parameters

Table S12 - Initial Lennard-Jones parameters for EC

Atom	R_{min} [a]	ε [b]
N	1.8240	0.1700
O	1.6612	0.2100
C_{ar}	1.9080	0.0860
H_{ar}	1.4590	0.0150
$C_{carbonyl}$	1.9080	0.0860
C_{al}	1.9080	0.1094
H_{al}	1.4870	0.0157

a - the distance where the potential reaches a minimum in Angstroms ($\sigma \times 2^{1/6}$), b - the potential well depth in kcal mol^{-1}

Table S13 Calculation of diffusion coefficients, their associated errors and ln D for 2,4-DNEB and NG-N1 in the NC, 2,4-DNEB and NG-N1 binder

	slope	std. error of slope	D	D	D std. error	D std. error	D	D	D std. error	T	1/T	ln D
	($Å^2$/ps)	($Å^2$/ps)	($Å^2$/ps)	(m^2/s)	($Å^2$/ps)	(m^2/s)	(cm^2/s)	(cm^2/s) 10^7	(cm^2/s)	(K)	(K)	(cm^2/s)
DNEB 298K	0.000987	0.0000188	0.000164467	1.645E-12	3.1333E-06	3.1333E-14	1.64E-08	0.164	3.13E-10	298	0.00336	-17.92
NGN1 298K	0.001109	3.38E-05	0.000184833	1.848E-12	5.6317E-06	5.6317E-14	1.85E-08	0.185	5.63E-10	298	0.00336	-17.81
DNEB 323K	0.002698	8.94E-05	0.000449667	4.497E-12	1.4902E-05	1.4902E-13	4.50E-08	0.450	1.49E-09	323	0.00310	-16.92
NGN1 323K	0.001301	1.855E-05	0.000216833	2.168E-12	3.0917E-06	3.0917E-14	2.17E-08	0.217	3.09E-10	323	0.00310	-17.65
DNEB 348K	0.005122	9.173E-05	0.000853667	8.537E-12	1.5288E-05	1.5288E-13	8.54E-08	0.854	1.53E-09	348	0.00287	-16.28
NGN1 348K	0.003381	3.94E-05	0.0005635	5.635E-12	6.5633E-06	6.5633E-14	5.64E-08	0.564	6.56E-10	348	0.00287	-16.69
DNEB 373K	0.00901	3.701E-05	0.001501667	1.502E-11	6.1683E-06	6.1683E-14	1.50E-07	1.502	6.17E-10	373	0.00268	-15.71
NGN1 373K	0.005754	2.14E-05	0.000959	9.59E-12	3.5717E-06	3.5717E-14	9.59E-08	0.959	3.57E-10	373	0.00268	-16.16
DNEB 398K	0.02027	5.199E-05	0.003378333	3.378E-11	8.665E-06	8.665E-14	3.38E-07	3.378	8.67E-10	398	0.00251	-14.90
NGN1 398K	0.01486	6.18E-05	0.002476667	2.477E-11	1.0302E-05	1.0302E-13	2.48E-07	2.477	1.03E-09	398	0.00251	-15.21

Table S14 Calculation of diffusion coefficients, their associated errors and ln D for 2,4-DNEB and 2,4,6-TNEB in the NC and K10 binder

	slope	std. error of slope	D	D	D std. error	D std. error	D	D	D std. error	T	1/T	ln D
	(Å2/ps)	(Å2/ps)	(Å2/ps)	(m2/s)	(Å2/ps)	(m2/s)	(cm2/s)	(cm2/s) 107	(cm2/s)	(K)	(K)	(cm2/s)
DNEB 298K	0.00198	1.63E-05	0.00032967	3.3E-12	2.7233E-06	2.72333E-14	3.30E-08	0.330	2.72E-10	298	0.00336	-17.23
TNEB 298K	0.00181	2.80E-05	0.000302	3E-12	4.6633E-06	4.66333E-14	3.02E-08	0.302	4.66E-10	298	0.00336	-17.32
DNEB 323K	0.01299	0.000312	0.002165	2.2E-11	0.000052	5.2E-13	2.17E-07	2.165	5.20E-09	323	0.00310	-15.35
TNEB 323K	0.00762	0.0001247	0.00127017	1.3E-11	2.0783E-05	2.07833E-13	1.27E-07	1.270	2.08E-09	323	0.00310	-15.88
DNEB 348K	0.02247	0.0002556	0.003745	3.7E-11	0.0000426	4.26E-13	3.75E-07	3.745	4.26E-09	348	0.00287	-14.80
TNEB 348K	0.01111	0.00008555	0.00185167	1.9E-11	1.4258E-05	1.42583E-13	1.85E-07	1.852	1.43E-09	348	0.00287	-15.50
DNEB 373K	0.02577	0.00005581	0.004295	4.3E-11	9.3017E-06	9.30167E-14	4.30E-07	4.295	9.30E-10	373	0.00268	-14.66
TNEB 373K	0.01845	0.00006755	0.003075	3.1E-11	1.1258E-05	1.12583E-13	3.08E-07	3.075	1.13E-09	373	0.00268	-14.99
DNEB 398K	0.05584	5.94E-05	0.00930667	9.3E-11	9.895E-06	9.895E-14	9.31E-07	9.307	9.90E-10	398	0.00251	-13.89
TNEB 398K	0.03454	0.00008873	0.00575667	5.8E-11	1.4788E-05	1.47883E-13	5.76E-07	5.757	1.48E-09	398	0.00251	-14.37

Table S15 Natural logarithms of the diffusion coefficients of 2,4-DNEB and 2,4 TNEB in an NC binder.

		ln D ($cm^2 s^{-1}$) for 2,4-DNEB and 2,4 TNEB in an NC binder	
T (K)	1/T (K)	2,4-DNEB	2,4,6-TNEB
298	0.00336	-17.23	-17.32
323	0.00310	-15.35	-15.88
348	0.00287	-14.80	-15.50
373	0.00268	-14.66	-14.99
398	0.00251	-13.89	-14.37

Table S16 Natural logarithms of the diffusion coefficients of 2,4-DNEB and NG-N1 in an NC binder.

		ln D ($cm^2 s^{-1}$) for 2,4-DNEB and NG-N1 in an NC binder	
T (K)	1/T (K)	2,4-DNEB	NG-N1
298	0.00336	-17.92	-17.81
323	0.00310	-16.92	-17.65
348	0.00287	-16.28	-16.69
373	0.00268	-15.71	-16.16
398	0.00251	-14.90	-15.21