

Supporting Information

Intermolecular interaction and mechanical properties of energetic plasticizer MNs reinforced 2,4,6- trinitrotoluene/1,3,5-trinitrohexahydro-1,3,5-triazine molten-energetic-composite(MEC)

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Page S2-S7: The Cartesian coordinates of all the optimized geometries along with the corresponding absolute energies and BSSE energies.

TNT+o-NT

C	4.454186	-1.118171	1.042122
C	3.091680	-1.311858	1.263639
C	2.268275	-0.190910	1.322000
C	2.776729	1.091956	1.136656
C	4.146225	1.232809	0.913977
C	5.053791	0.148848	0.849656
N	5.281057	-2.365018	1.026645
H	2.681968	-2.308741	1.385111
N	0.811072	-0.369212	1.573869
H	2.122953	1.957520	1.156389
N	4.626830	2.640081	0.749483
C	6.517825	0.321888	0.521905
H	6.917754	-0.565322	0.025053
H	7.097870	0.475670	1.440667
H	6.678043	1.194208	-0.117186
O	4.792118	-3.358243	0.455247
O	6.382067	-2.330943	1.608644
O	0.388450	-1.537665	1.682844
O	0.114793	0.660914	1.654189
O	3.900740	3.410977	0.094465
O	5.701820	2.946813	1.300122
C	-5.135569	-1.570779	-0.981208
C	-6.454417	-1.689077	-1.428478
C	-7.143271	-0.560377	-1.891959
C	-6.495027	0.672770	-1.905067
C	-5.177709	0.776964	-1.433867
C	-4.449497	-0.340174	-0.958043
H	-6.941487	-2.663277	-1.418648
H	-6.987635	1.569226	-2.268595
N	-4.580819	2.138457	-1.472480
C	-3.019436	-0.311756	-0.467021
H	-2.645233	-1.335806	-0.355121
H	-2.936290	0.195900	0.501364
H	-2.360454	0.232834	-1.153373
O	-5.071708	2.966409	-2.272513
O	-3.630934	2.392620	-0.699616
H	-4.606328	-2.458991	-0.638472
H	-8.170431	-0.640543	-2.242399

Sum of electronic and zero-point Energies= -1361.39964825

Counterpoise: corrected energy = -1357.973619122889

Counterpoise: BSSE energy = 0.001592560627

TNT+p-NT

C	4.433524	0.718563	-0.786142
C	3.066468	0.639690	-0.524248
C	2.452972	-0.608018	-0.592838
C	3.181127	-1.757840	-0.886065
C	4.545741	-1.627413	-1.138028
C	5.245790	-0.398073	-1.097345
N	5.015003	2.096012	-0.729867
H	2.496196	1.526552	-0.270426
N	0.991817	-0.717214	-0.331268
H	2.700565	-2.730034	-0.911721
N	5.258051	-2.899469	-1.473101
C	6.741949	-0.301024	-1.279230
H	6.988578	-0.127353	-2.334424
H	7.235457	-1.226961	-0.973520
H	7.153928	0.532540	-0.705006
O	4.594205	2.849270	0.168596
O	5.852823	2.400423	-1.600127
O	0.382009	0.332414	-0.044924
O	0.477361	-1.850043	-0.413056
O	4.940327	-3.911438	-0.819912
O	6.094503	-2.862385	-2.395427
C	-5.675988	-0.667806	1.107475
C	-6.747277	0.225207	1.115173
C	-6.479836	1.599180	1.144968
C	-5.168884	2.085849	1.167441
C	-4.110436	1.175307	1.157503
C	-4.341393	-0.213337	1.124998
H	-7.777329	-0.117430	1.101354
H	-4.996619	3.157600	1.193700
C	-3.192349	-1.194520	1.087796
H	-3.397395	-2.073169	1.713738
H	-2.255639	-0.736569	1.424967
H	-3.021985	-1.557313	0.063226
H	-5.877353	-1.738643	1.088142
N	-7.608622	2.557413	1.154622
O	-8.770916	2.093925	1.129684
O	-7.339657	3.779260	1.185850
H	-3.086716	1.546843	1.177443

Sum of electronic and zero-point Energies= -1361.40598501

Counterpoise: corrected energy = -1357.976442558212

Counterpoise: BSSE energy = 0.001197883074

RDX+o-NT

C	3.404683	0.866053	0.960342
C	4.518116	1.179638	1.745986
C	5.737296	0.524099	1.531815
C	5.823920	-0.445189	0.533848
C	4.702072	-0.737228	-0.257155
C	3.456617	-0.088616	-0.074438
H	4.429955	1.932046	2.528167
H	6.746855	-0.984827	0.346953
N	4.896314	-1.778657	-1.301101
C	2.198765	-0.359275	-0.871230
H	2.309094	-0.029962	-1.911610
H	1.360131	0.177821	-0.414524
H	1.960255	-1.429271	-0.911262
O	5.861568	-2.563336	-1.167743
O	4.096488	-1.815468	-2.262996
H	2.457285	1.368570	1.148650
H	6.609901	0.760612	2.137768
C	-4.930236	0.203500	-0.268279
N	-4.236162	-1.078617	-0.297178
C	-3.074270	-1.204933	0.570405
N	-2.107270	-0.105821	0.250514
C	-2.540346	0.927541	-0.709247
N	-3.946916	1.306424	-0.515682
H	-5.376877	0.335018	0.723211
H	-5.717669	0.209245	-1.022269
N	-4.147968	-1.750210	-1.609628
H	-2.607869	-2.179558	0.425889
H	-3.406083	-1.111078	1.610580
N	-1.215500	0.248618	1.289874
H	-2.422862	0.533380	-1.724450
H	-1.911301	1.808767	-0.584608
N	-4.231693	2.542878	0.140853
O	-3.306884	-2.649519	-1.703631
O	-4.970020	-1.392449	-2.459399
O	-1.150088	-0.559763	2.236555
O	-0.543682	1.285348	1.143402
O	-5.400337	2.666641	0.553125
O	-3.325282	3.387578	0.188491

Sum of electronic and zero-point Energies= -1373.78831063

Counterpoise: corrected energy = -1370.361915490549

Counterpoise: BSSE energy = 0.002966408057

RDX+p-NT

C	4.118615	-1.373393	1.927772
C	5.503465	-1.223118	1.829783
C	6.027537	0.046612	1.565116
C	5.195564	1.159996	1.403354
C	3.814103	0.988156	1.504757
C	3.249815	-0.276972	1.764960
H	6.177718	-2.064485	1.957269
C	1.749794	-0.452403	1.842759
H	1.473508	-1.306879	2.472501
H	1.329093	-0.632785	0.841463
H	1.258137	0.443136	2.241903
H	3.704076	-2.359159	2.136802
N	7.495287	0.216012	1.454807
H	3.160322	1.851281	1.382718
H	5.636888	2.132138	1.205906
O	8.213840	-0.797093	1.604696
O	7.934465	1.362673	1.215340
C	-4.991746	0.275412	-1.442994
N	-4.480523	-0.987689	-1.959706
C	-3.287143	-1.535151	-1.290643
N	-2.390883	-0.430863	-0.854636
C	-2.526092	0.825214	-1.601364
N	-3.924911	1.311515	-1.591682
H	-5.253605	0.125524	-0.387202
H	-5.879908	0.576454	-1.995349
N	-4.536567	-1.143711	-3.421142
H	-2.774041	-2.190266	-1.996823
H	-3.577923	-2.104354	-0.404501
N	-2.180776	-0.310528	0.576975
H	-2.217791	0.616615	-2.631885
H	-1.884959	1.597508	-1.178477
N	-4.196273	2.562266	-0.971835
O	-3.832169	-2.040270	-3.904545
O	-5.336788	-0.414525	-4.015514
O	-2.361510	-1.339079	1.248192
O	-1.769054	0.784725	0.985382
O	-5.374731	2.728090	-0.603270
O	-3.264837	3.379394	-0.910890

Sum of electronic and zero-point Energies= -1373.79359441

Counterpoise: corrected energy = -1370.364915331080

Counterpoise: BSSE energy = 0.001780888389

TNT+RDX

C	3.536703	1.256685	0.543252
C	4.875649	1.273899	0.152945
C	5.534929	0.056756	0.007801
C	4.893326	-1.149326	0.272458
C	3.555475	-1.113942	0.666890
C	2.811420	0.077889	0.834501
N	2.877710	2.597159	0.624330
H	5.388444	2.211370	-0.033891
N	6.960813	0.045613	-0.429467
H	5.420050	-2.092489	0.174797
N	2.922210	-2.449322	0.896882
C	1.394129	0.094192	1.356916
H	1.214077	-0.748579	2.029613
H	0.682189	0.009158	0.526608
H	1.175615	1.025798	1.883665
O	3.549499	3.529495	1.102962
O	1.718378	2.691540	0.176049
O	7.503595	1.148757	-0.630597
O	7.507744	-1.066052	-0.561435
O	3.622978	-3.320513	1.444754
O	1.751923	-2.606115	0.496649
C	-5.116795	-0.154665	-0.809479
N	-4.327052	-1.301388	-1.238308
C	-3.147573	-1.627283	-0.420112
N	-2.512851	-0.380784	0.092800
C	-2.788560	0.833578	-0.686538
N	-4.244023	1.057887	-0.845290
H	-5.472862	-0.353573	0.209692
H	-5.971420	-0.015846	-1.469267
N	-4.175014	-1.456700	-2.693434
H	-2.445203	-2.186319	-1.040870
H	-3.441555	-2.234060	0.439773
N	-2.495583	-0.227255	1.538994
H	-2.331341	0.687648	-1.671422
H	-2.350651	1.709277	-0.208463
N	-4.808409	2.233355	-0.275717
O	-3.266331	-2.207500	-3.072825
O	-5.015379	-0.882380	-3.393066
O	-2.593988	-1.269314	2.205615
O	-2.304490	0.919052	1.967942
O	-6.033120	2.179655	-0.052000
O	-4.054655	3.204640	-0.113709

Sum of electronic and zero-point Energies= -1782.94851711

Counterpoise: corrected energy = -1778.559914613296

Counterpoise: BSSE energy = 0.003484801495