Supporting Information

Comparative study on melting points of 3,4-bis(3-nitrofurazan-4-yl)furoxan(DNTF)/1,3,3-trinitroazetidine (TNAZ) eutectic compositions with molecular dynamic simulations

Ning Liu,* Svatopluk Zeman, Yuan-jie Shu, Zong-kai Wu, Bo-zhou Wang, and Shi-wei Yin

Email: flackliu@sina.com

Table S1 The calculated specific volume of DNTF and TNAZ at different temperatures[a]

Compound	Specific volume/cm^3 g^{-1}	Temperature/K
DNTF	0.5387	280
	0.5410	300
	0.5428	320
	0.5436	340
	0.5447	360
	0.5463	380
	0.5475	400
	0.5536	420
	0.5562	440
	0.5610	460
	0.5655	480
	0.5677	500
TNAZ	0.5883	260
	0.5907	280
	0.5972	300
	0.6002	320
	0.6110	340
	0.6204	360
	0.6277	380
	0.6410	400
	0.6501	420
	0.6690	440
	0.6799	460
	0.6978	480

[a] The data in Table S1 correspond to Fig. 3 and Fig. 4.

Table S2 The calculated specific volume of DNTF/TNAZ eutectic compositions at different temperatures[a]

Composition	Specific volume/cm^3 g^{-1}	Temperature /K	Composition	Specific volume/cm^3 g^{-1}	Temperature /K
mixture 1	0.5702	260	mixture 2	0.5651	240
	0.5768	280		0.5681	260
	0.5793	300		0.5707	280
	0.5837	320		0.5747	300
	0.5909	340		0.5790	320
	0.5981	360		0.5848	340
	0.6060	380		0.5897	360
	0.6175	400		0.5966	380
	0.6264	420		0.6077	400
	0.6373	440		0.6177	420
	0.6492	460		0.6235	440
	0.6597	480		0.6363	460
mixture 3	0.5623	240	mixture 4	0.5583	240
	0.5634	260		0.5594	260
	0.5684	280		0.5623	280
	0.5707	300		0.5652	300
	0.5742	320		0.5691	320
	0.5792	340		0.5714	340
	0.5848	360		0.5747	360
	0.5899	380		0.5813	380
	0.5971	400		0.5866	400
	0.6039	420		0.5914	420
	0.6140	440		0.5992	440
	0.6238	460		0.6058	460
mixture 5	0.5512	260			
	0.5560	280			
	0.5595	300			
	0.5624	320			
	0.5644	340			
	0.5668	360			
	0.5720	380			
	0.5788	400			
	0.5835	420			
	0.5903	440			
	0.5953	460			
	0.6005	480			

[a] The data in Table S2 correspond to Fig. 5.

Table S3 The free volume of mixture 3 at different temperatures[a]

Free volume/Å^3	Temperature/K
1238.83	240
1254.80	260
1289.82	280
1296.55	300
1333.47	320
1376.60	340
1454.31	360
1690.18	380
1916.24	400
2119.19	420
2472.13	440
2679.71	460

[a] The data in Table S3 correspond to Fig. 6.

Table S4 The diffusion coefficient of mixture 3 at different temperatures[a]

Diffusion coefficient/$\times 10^{-11}$ m^2 s^{-1}	Temperature/K
0.498	240
0.622	260
1.079	280
1.315	300
1.545	320
2.455	340
3.462	360
4.547	380
6.848	400
8.982	420
10.514	440
12.564	460

[a] The data in Table S4 correspond to Fig. 8.

Table S5 The specific heat capacity of mixture 3 at different temperatures[a]

Specific heat capacity/J g^{-1} K^{-1}	Temperature/K
0.912	240
0.985	260
1.013	280
1.060	300
1.137	320
1.194	340
1.228	360
1.252	380
1.309	400
1.331	420
1.350	440
1.396	460

[a] The data in Table S5 correspond to Fig. 9.

Table S6 The non-bonded energy of mixture 3 at different temperatures[a]

Non-bonded energy /kcal mol^{-1}	Temperature/K
−7201.76	240
−7198.70	260
−7170.27	280
−7151.07	300
−7145.17	320
−7104.17	340
−7075.89	360
−7057.68	380
−6990.71	400
−6966.67	420
−6924.78	440
−6845.63	460

[a] The data in Table S6 correspond to Fig. 10.
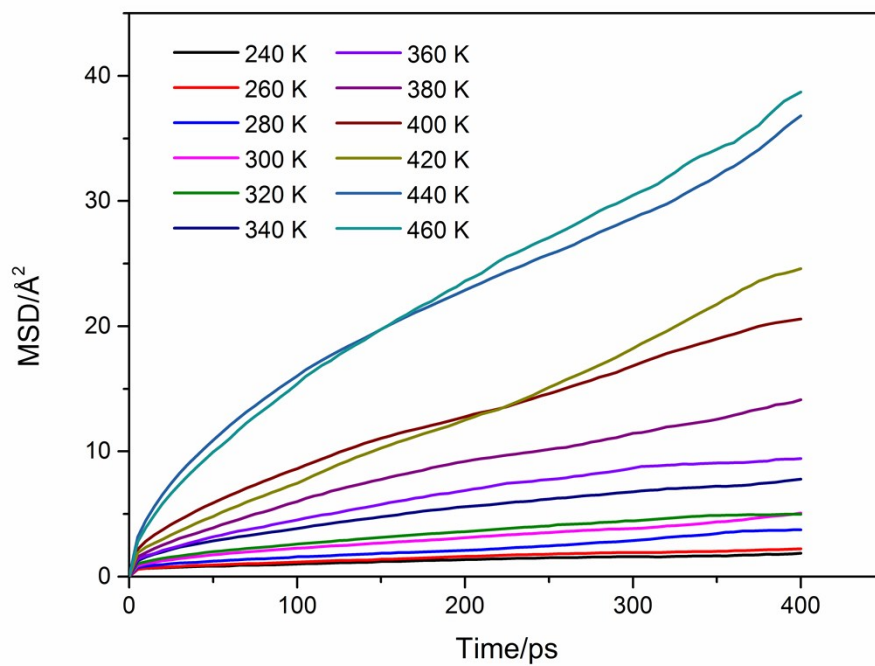
Fig. S1 The mean square displacement versus time curves for mixture 3 at temperatures from 240 K to 460 K.