

Electronic supplementary information for

Synthesis, characterization and properties of 1, 2, 8, 9-tetraazido-4, 6-dioxol-nonane: A promising multi-azido ether energetic plasticizer for GAP

Ruoqian Xu,^{*a, b} Zhongming Li,^{*b, c} Yanhui Chen,^b Yinglei Wang^a and Baodong Zhao^a

^a Xi'an Modern Chemistry Research Institute, Xi'an 710065, China. E-mail: xurq204@163.com; Tel: +86-029-88291556.

^b School of Science, Northwestern Polytechnical University, Xi'an 710129, China. E-mail: lizm_nwpu@163.com

^c Sichuan University, Chengdu 610065, China.

Contents

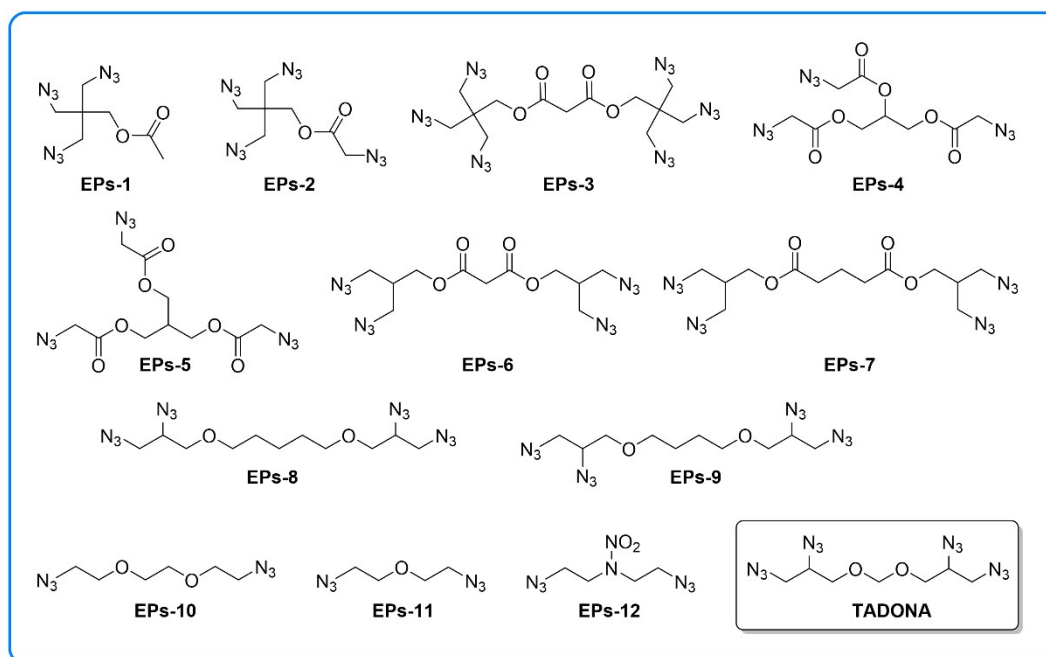
Scheme S1 Partial energetic plasticizers designed in this work during the preliminary screening.

Table S1 Theoretical calculated properties of partial energetic plasticizers designed in this work

Fig. S1 DSC thermograms of the thermal decomposition of TADONA under various heating rates.

Fig. S2 Kinetic plots for TADONA by the Kissinger method.

Fig. S3 Kinetic plots for TADONA by the Ozawa method.



Scheme S1 Partial energetic plasticizers designed in this work during the preliminary screening.

Table S1 Theoretical calculated properties of partial energetic plasticizers designed in this work

	Formula	M/g·mol ⁻¹	N/% ^c	OB/% ^d	ρ /g·cm ^{-3e}	ΔH_f /kJ·mol ⁻¹ⁱ	T_g /°C ^h
EPs-1	C ₇ H ₁₁ N ₉ O ₂	253.23	49.78	-110.57	1.25	595.36	-73.8
EPs-2	C ₇ H ₁₀ N ₁₂ O ₂	294.24	57.12	-92.44	1.32	1725.00	-50.4
EPs-3	C ₁₃ H ₁₈ N ₁₈ O ₄	490.41	51.41	-101.14	1.35	1305.89	-58.3
EPs-4	C ₉ H ₁₁ N ₉ O ₆	341.24	36.94	-82.05	1.54	649.17	-70.5
EPs-5	C ₁₀ H ₁₃ N ₉ O ₆	355.27	35.48	-92.32	1.45	730.54	-34.1
EPs-6	C ₁₁ H ₁₆ N ₁₂ O ₄	380.33	44.19	-109.38	1.25	581.62	-69.4
EPs-7	C ₁₃ H ₂₀ N ₁₂ O ₄	408.38	41.16	-125.37	1.27	550.75	-68.5
EPs-8	C ₁₁ H ₂₀ N ₁₂ O ₂	352.36	47.70	-136.22	1.32	834.58	-82.3
EPs-9	C ₁₀ H ₁₈ N ₁₂ O ₂	338.34	49.68	-127.68	1.33	804.19	-86.4
EPs-10	C ₆ H ₁₂ N ₆ O ₂	200.20	41.98	-127.87	1.13	898.1	-62.2
EPs-11	C ₄ H ₈ N ₆ O	156.15	53.82	-112.71	1.14	912.5	-58.4
EPs-12	C ₄ H ₈ N ₈ O ₂	200.16	55.98	-79.64	1.33	539.2	-38.0
TADONA	C ₇ H ₁₂ N ₁₂ O ₂	296.26	56.74	-97.21	1.32	857.3	-92.3

^a Nitrogen content in mass %; ^b Oxygen balance (based on CO₂) for C_aH_bO_cN_d, 1600(c-2a-b/2)/MW, MW=molecular weight; ^c Density; ^d Heat of formation; ^e Glass transition temperature.

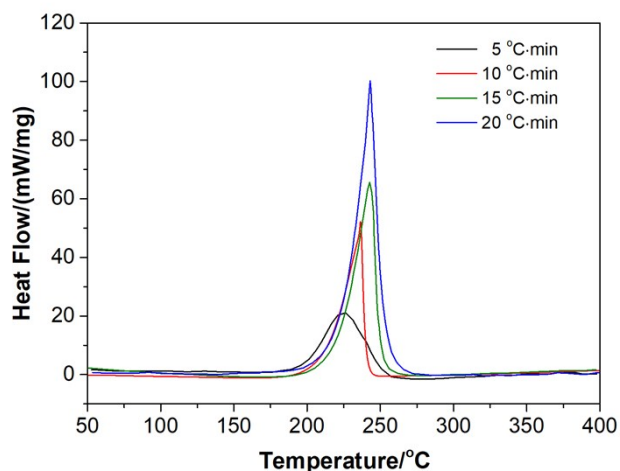


Fig. S1 DSC thermograms of the thermal decomposition of TADONA under various heating rates.

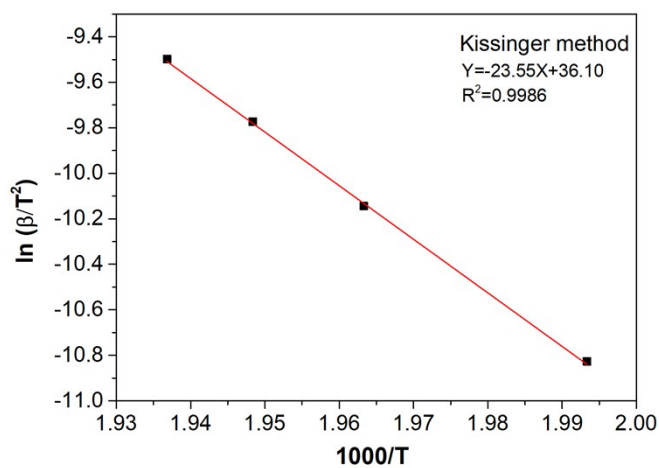


Fig. S2 Kinetic plots for TADONA by Kissinger method.

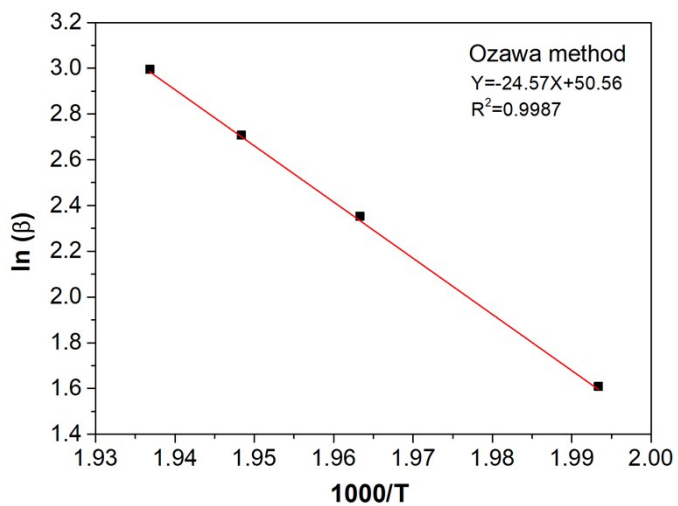


Fig. S3 Kinetic plots for TADONA by Ozawa method.