

Supporting Materials

For

Multi-step Thermolysis Mechanisms of Azido-s-triazine Derivatives and Kinetic Compensation Effect for the Rate-limiting Processes

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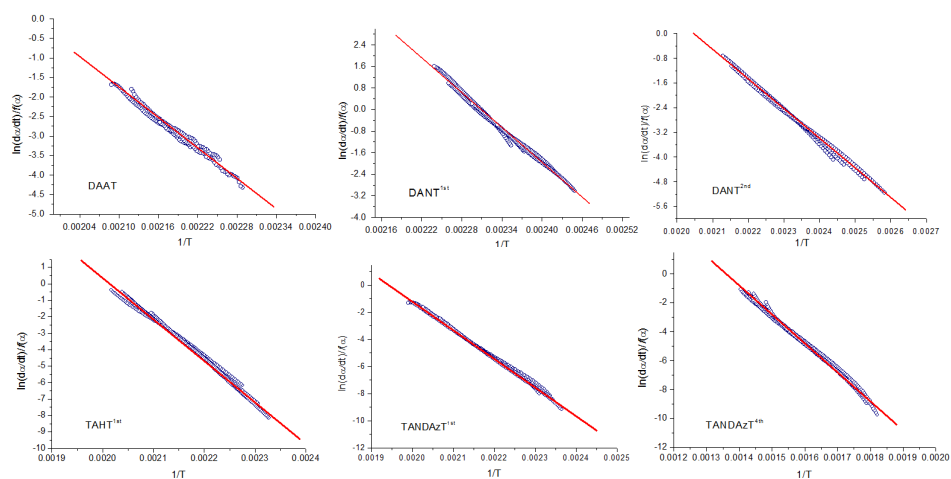


Fig. S1 Selected combined kinetic analysis plots for non-isothermal decomposition data of DAAT, DANT, THAT and TANDAzT

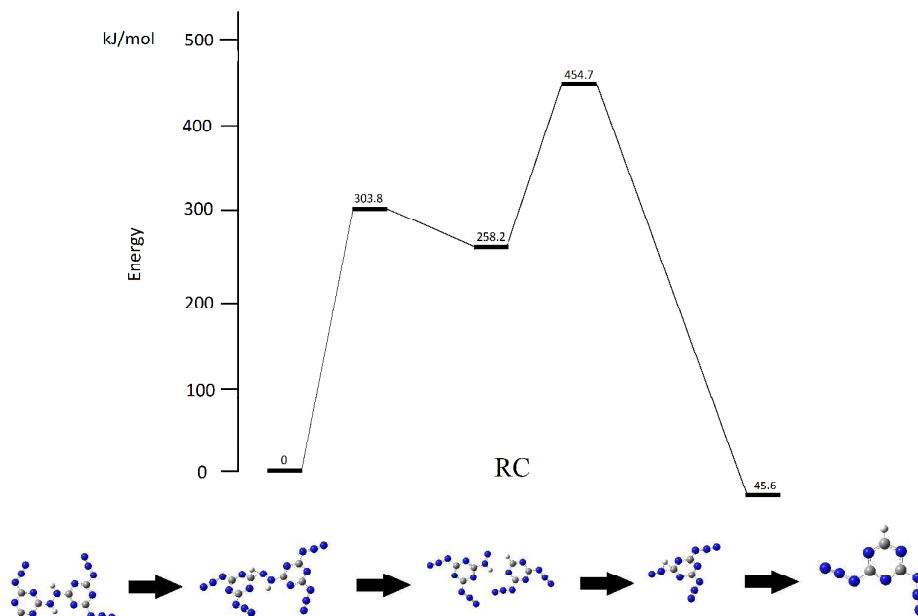


Fig. S2 Energy barriers for initial decomposition pathways of TAHT

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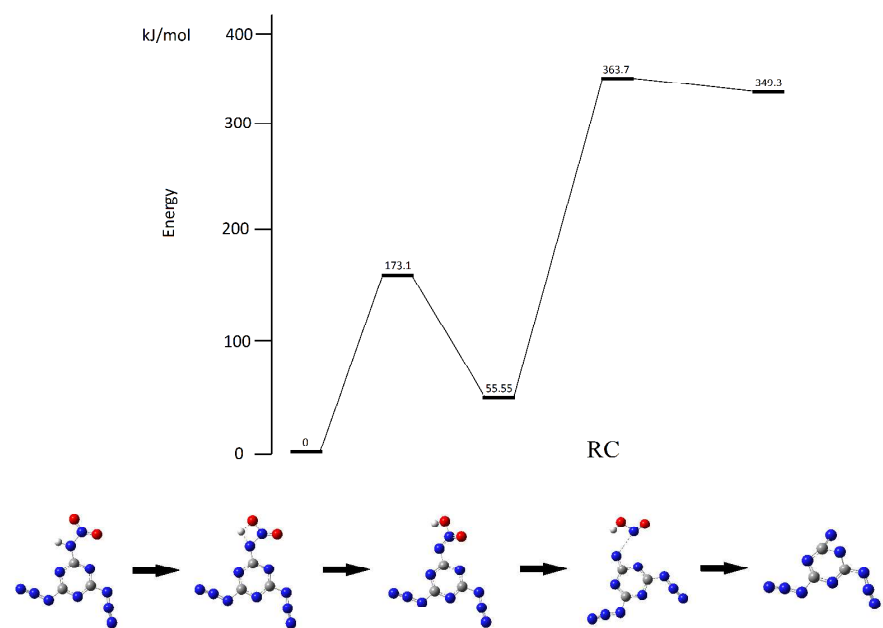


Fig. S3 Energy barriers for initial decomposition pathways of DANT

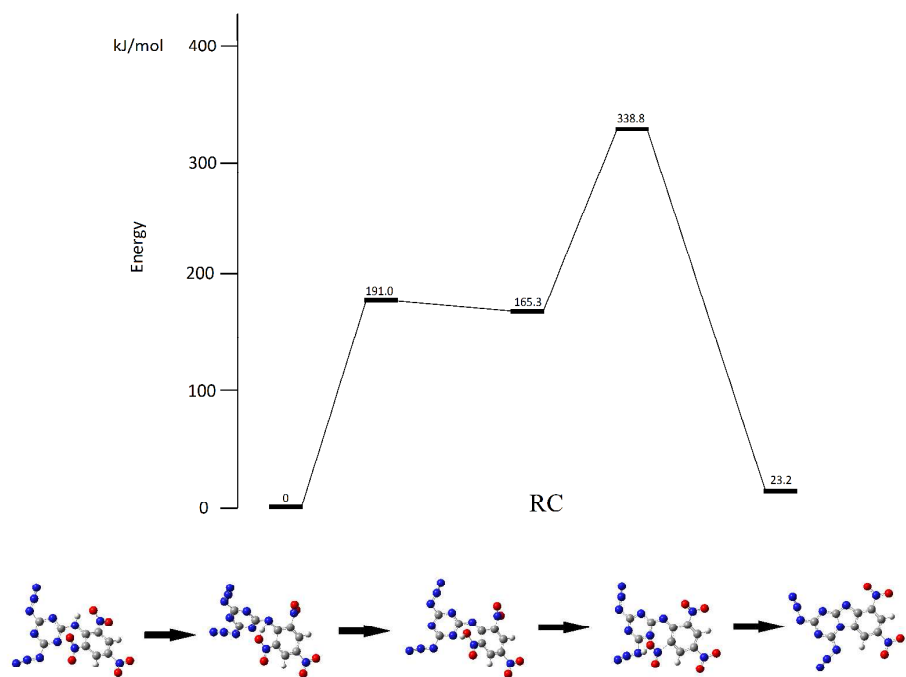


Fig. S4 Energy barriers for initial decomposition pathways of TANDAzT

Table S1 Kinetic data of DAAT and DANT by Friedman's isoconversional method

α reacted	DANT-1 st		DANT-2 nd		DANT-3 rd		DANT-4 th		DAAT	
	E_a	r	E_a	r	E_a	r	E_a	r	E_a	r
0.10	166.4	0.9982	75.0	0.9978	134.0	0.9886	124.4	0.9999	90.5	0.9455
0.20	172.3	0.9982	77.9	0.9967	133.9	0.9894	129.5	1.0000	93.9	0.9695
0.30	176.1	0.9978	79.7	0.9959	133.7	0.9900	132.9	0.9999	97.9	0.9786
0.40	179.1	0.9974	81.2	0.9953	133.4	0.9904	135.6	0.9998	92.3	0.9868
0.50	181.7	0.9970	82.4	0.9948	133.0	0.9907	137.9	0.9997	98.8	0.9950
0.60	184.0	0.9965	83.4	0.9945	132.5	0.9909	140.1	0.9997	103.8	0.9966
0.70	186.3	0.9962	84.4	0.9942	131.8	0.9911	142.1	0.9996	107.2	0.9978
0.80	188.5	0.9958	85.3	0.9942	130.9	0.9910	144.1	0.9995	114.4	0.9955
0.90	190.8	0.9956	86.1	0.9946	129.2	0.9905	146.3	0.9996	115.7	0.9916
Mean^b	181.2±10 kJ mol ⁻¹		82.1±6 kJ mol ⁻¹		132±1 kJ mol ⁻¹		137.7±2 kJ mol ⁻¹		101.6±8 kJ mol ⁻¹	

Table S2 Kinetic data of TAHT and TANDAzT by Friedman's isoconversional method

α reacted	TAHT-1 st		TAHT-2 nd		TANDAzT-1 st		TANDAzT-2 nd		TANDAzT-3 rd		TANDAzT-4 th	
	E_a	r	E_a	r	E_a	r	E_a	r	E_a	r	E_a	r
0.10	203.5	0.9998	163.1	0.9986	179.4	0.9994	122.7	0.9943	140.6	0.9981	164.4	0.9778
0.20	194.4	0.9998	164.7	0.9985	177.5	0.9992	125.9	0.9937	115.9	0.9982	161.2	0.9792
0.30	188.6	0.9991	166.1	0.9986	176.0	0.9976	127.7	0.9933	101.6	0.9988	159.9	0.9800
0.40	184.0	0.9982	167.5	0.9986	174.5	0.9960	128.8	0.9932	91.4	0.9995	159.0	0.9806
0.50	180.0	0.9971	168.8	0.9987	172.7	0.9948	129.6	0.9932	83.3	0.9999	158.0	0.9810
0.60	176.3	0.9958	170.4	0.9988	170.2	0.9939	130.2	0.9933	76.4	0.9999	156.6	0.9814
0.70	172.7	0.9942	172.1	0.9989	166.7	0.9937	130.6	0.9936	70.3	0.9988	154.3	0.9817
0.80	168.9	0.9921	174.4	0.9989	161.1	0.9944	131.0	0.9941	64.6	0.9958	150.5	0.9819
0.90	164.4	0.9891	177.8	0.9989	149.5	0.9956	131.1	0.9949	59.1	0.9881	142.1	0.9819
Mean^b	181.4±9 kJ mol ⁻¹		169.4±6 kJ mol ⁻¹		169.7±10 kJ mol ⁻¹		128.6±10 kJ mol ⁻¹		89.2±3 kJ mol ⁻¹		156.2±8 kJ mol ⁻¹	