

Supporting information:

Thermal Behavior of Nitrocellulose-Based Superthermites: Effects of nano-Fe₂O₃ with three morphologies

Ting Zhang^a, Ningning Zhao^a, Jiachen Li^a, Hujun Gong^b, Ting An^c, Fengqi Zhao^c, Haixia Ma^{a,*}

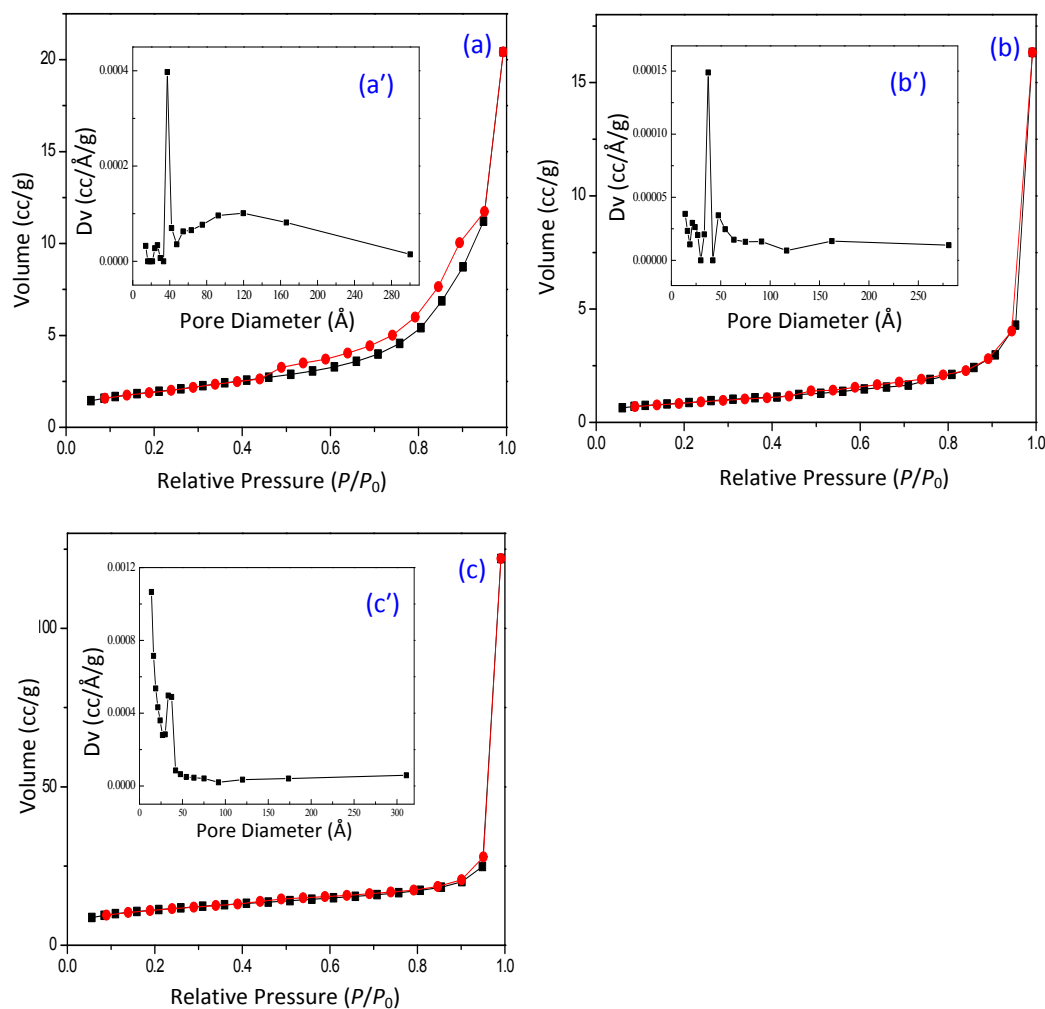


Fig.S1 Nitrogen adsorption-desorption isotherms and pore size distribution curves (inset) of the samples. (a,a') Fe₂O₃(p); (b,b') Fe₂O₃(o); (c,c') Fe₂O₃(r).

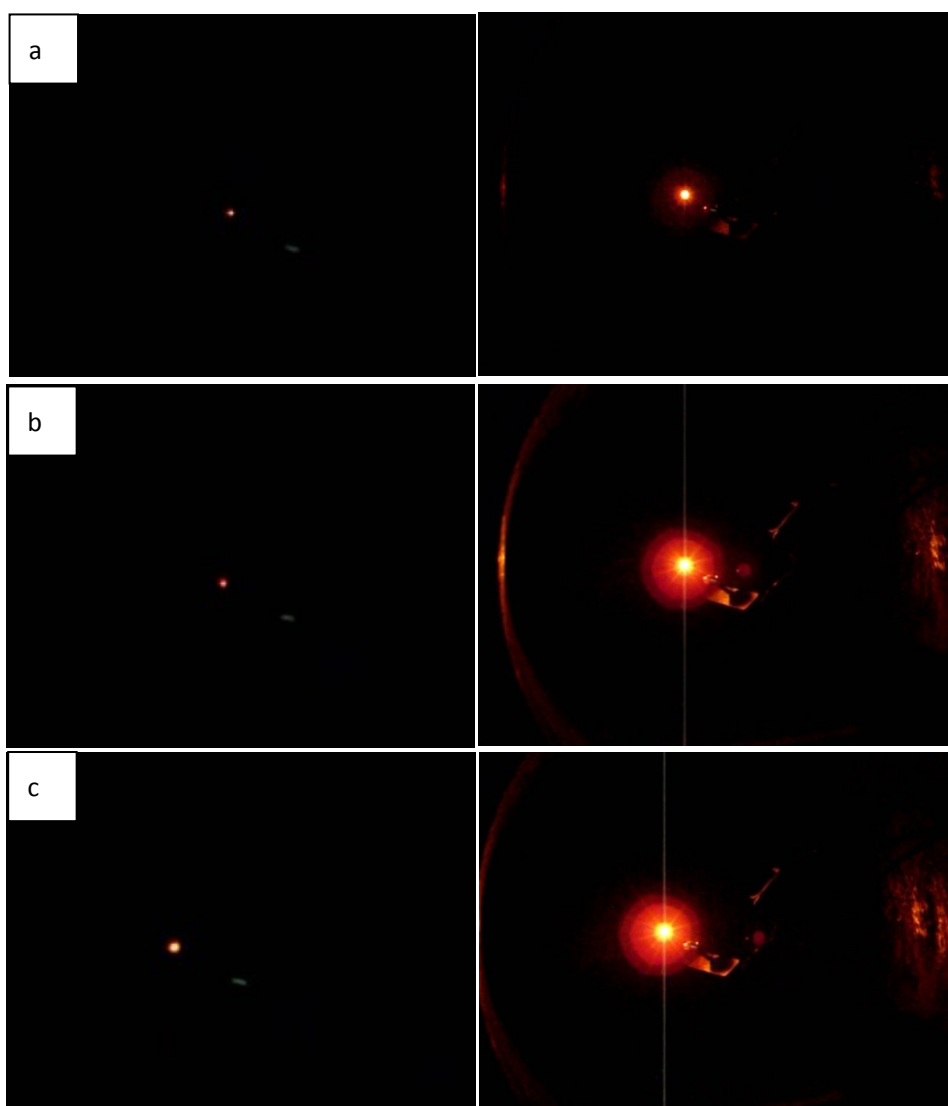


Fig.S2 The initial (left) and final (right) sparkle taken from the laser ignition process video for the three particles (a) $\text{Fe}_2\text{O}_3(\text{p})$; (b) $\text{Fe}_2\text{O}_3(\text{o})$; (c) $\text{Fe}_2\text{O}_3(\text{r})$.

Table S1 Calculated values of kinetic parameters of decomposition reaction for NC-Al/Fe₂O₃(r)

Method	$\beta/ ^\circ\text{C}/\text{min}$	$E_a/\text{kJ}/\text{mol}$	$\log(A/\text{s}^{-1})$	r	S	d
MacCallum-Tanner	5	176.94	17.05	0.9929	5.58×10^{-3}	4.64×10^{-5}
	10	185.02	17.99	0.9946	5.06×10^{-3}	2.74×10^{-5}
	15	179.24	17.37	0.9942	5.38×10^{-3}	3.10×10^{-5}
	20	195.19	19.12	0.9957	3.99×10^{-3}	1.71×10^{-5}
	25	179.49	17.41	0.9954	4.30×10^{-3}	1.98×10^{-5}
	30	186.06	18.11	0.9949	4.75×10^{-3}	2.41×10^{-5}
Šatava-Šesták	5	175.24	16.90	0.9929	6.58×10^{-3}	4.64×10^{-5}
	10	182.87	17.80	0.9946	5.06×10^{-3}	2.74×10^{-5}
	15	177.41	17.21	0.9942	5.38×10^{-3}	3.10×10^{-5}
	20	192.47	18.87	0.9957	3.99×10^{-3}	1.71×10^{-5}
	25	177.65	17.25	0.9954	4.30×10^{-3}	1.98×10^{-5}
	30	183.85	17.91	0.9949	4.75×10^{-3}	2.41×10^{-5}
Agrawal	5	176.35	17.03	0.9923	3.50×10^{-2}	2.70×10^{-4}
	10	184.27	17.95	0.9941	2.69×10^{-2}	1.59×10^{-4}
	15	178.47	17.33	0.9937	2.86×10^{-2}	1.81×10^{-4}
	20	194.26	19.05	0.9954	2.12×10^{-2}	9.87×10^{-4}
	25	178.63	17.36	0.9950	2.29×10^{-2}	1.15×10^{-4}
	30	185.12	18.05	0.9944	2.52×10^{-2}	1.40×10^{-4}
General integral	5	176.35	17.03	0.9923	3.50×10^{-2}	2.70×10^{-4}
	10	184.27	17.95	0.9941	2.69×10^{-2}	1.59×10^{-4}
	15	178.47	17.33	0.9937	2.86×10^{-2}	1.81×10^{-4}
	20	194.26	19.05	0.9954	2.12×10^{-2}	9.87×10^{-4}
	25	178.63	17.36	0.9950	2.29×10^{-2}	1.15×10^{-4}
	30	185.12	18.05	0.9944	2.52×10^{-2}	1.40×10^{-4}
Universal integral	5	175.00	15.59	0.9922	3.49×10^{-2}	2.72×10^{-4}
	10	183.06	16.50	0.9940	2.68×10^{-2}	1.60×10^{-4}
	15	177.35	15.90	0.9936	2.85×10^{-2}	1.82×10^{-4}
	20	193.20	17.60	0.9953	2.12×10^{-2}	9.91×10^{-4}
	25	177.62	15.95	0.9949	2.28×10^{-2}	1.16×10^{-4}
	30	184.15	16.62	0.9944	2.51×10^{-2}	1.41×10^{-4}
Mean		182.53	17.49			
Flynn-Wall-Ozawa		184.90(E_{eo})		0.9977	1.88×10^{-3}	
		184.27(E_{po})		0.9882	9.75×10^{-3}	

Kissinger	185.70(E_K)	18.31	0.9871	5.18×10 ⁻²
Mean(E_{eo} , E_{po} , E_K)	184.96			

Note: E with the subscript of eo and po is the apparent activation energy obtained from the onset temperature (T_o) and the peak temperature (T_p) by Ozawa's method, E with the subscript of K is the apparent activation energy obtained from the peak temperature (T_p) by Kissinger's method.

Table S2 Calculated values of kinetic parameters of decomposition reaction for NC-Al/Fe₂O₃(p).

Method	$\beta/^\circ\text{C min}^{-1}$	$E_a/\text{kJ mol}^{-1}$	$\log(A/\text{s}^{-1})$	r	S	d
MacCallum-Tanner	5	180.51	17.49	0.9827	5.70×10 ⁻²	9.88×10 ⁻⁴
	10	181.71	17.64	0.9825	5.76×10 ⁻²	1.01×10 ⁻⁴
	15	196.58	19.32	0.9856	4.74×10 ⁻²	6.33×10 ⁻⁴
	20	195.91	19.22	0.9864	4.48×10 ⁻²	6.11×10 ⁻⁴
	25	197.95	19.43	0.9871	4.24×10 ⁻²	5.45×10 ⁻⁴
	30	205.39	20.24	0.9862	4.56×10 ⁻²	6.31×10 ⁻⁴
Šatava-Šesták	5	178.61	17.32	0.9827	5.70×10 ⁻²	9.88×10 ⁻⁴
	10	179.75	17.47	0.9825	5.76×10 ⁻²	1.01×10 ⁻⁴
	15	193.78	19.05	0.9856	4.74×10 ⁻²	6.83×10 ⁻⁴
	20	193.16	18.96	0.9864	4.48×10 ⁻²	6.11×10 ⁻⁴
	25	195.08	19.16	0.9871	4.24×10 ⁻²	5.45×10 ⁻⁴
	30	202.11	19.93	0.9862	4.56×10 ⁻²	6.31×10 ⁻⁴
Agrawal	5	179.91	17.46	0.9811	3.03×10 ⁻¹	5.73×10 ⁻³
	10	181.00	17.61	0.9809	3.06×10 ⁻¹	5.84×10 ⁻³
	15	195.70	19.25	0.9844	2.52×10 ⁻²	3.94×10 ⁻⁴
	20	194.99	19.16	0.9852	2.38×10 ⁻¹	3.53×10 ⁻³
	25	196.97	19.35	0.9860	2.25×10 ⁻¹	3.15×10 ⁻³
	30	204.33	20.15	0.9850	2.42×10 ⁻¹	3.63×10 ⁻³
General integral	5	178.54	16.01	0.9809	3.02×10 ⁻¹	5.77×10 ⁻³
	10	179.78	16.17	0.9807	3.05×10 ⁻¹	5.88×10 ⁻³
	15	194.55	17.79	0.9843	2.51×10 ⁻¹	3.96×10 ⁻⁴
	20	193.91	17.70	0.9851	2.38×10 ⁻¹	3.54×10 ⁻³
	25	195.94	17.90	0.9859	2.25×10 ⁻¹	3.16×10 ⁻³
	30	203.34	18.68	0.9849	2.42×10 ⁻¹	3.64×10 ⁻³
Universal integral	5	179.91	17.47	0.9811	3.03×10 ⁻¹	5.73×10 ⁻³
	10	181.00	17.61	0.9809	1.79×10 ⁻¹	1.69×10 ⁻³
	15	195.70	19.26	0.9844	2.52×10 ⁻¹	3.94×10 ⁻⁴
	20	194.99	19.16	0.9852	2.38×10 ⁻¹	3.53×10 ⁻³
	25	196.97	19.35	0.9860	2.25×10 ⁻¹	3.15×10 ⁻³

	30	204.33	20.15	0.9850	2.42×10^{-1}	3.63×10^{-3}
Mean		191.75	18.51			
Flynn-Wall-Ozawa		178.20(E_{eo})		0.9996		
		190.08(E_{po})		0.9957		
Kissinger		191.83(E_K)	19.02	0.9953		
Mean(E_{eo}, E_{po}, E_K)		186.70				

Note: E with the subscript of eo and po is the apparent activation energy obtained from the onset temperature (T_e) and the peak temperature (T_p) by Ozawa's method, E with the subscript of K is the apparent activation energy obtained from the peak temperature (T_p) by Kissinger's method.

Table S3 Calculated values of kinetic parameters of decomposition reaction for NC-Al/Fe₂O₃(o).

Method	$\beta / ^\circ\text{C min}^{-1}$	$E_a / \text{kJ mol}^{-1}$	$\log(A/\text{s}^{-1})$	r	S	d
MacCallum-Tanner	5	176.67	17.03	0.9907	1.81×10^{-2}	1.68×10^{-4}
	10	185.48	18.02	0.9926	1.44×10^{-2}	1.07×10^{-4}
	15	191.71	18.72	0.9945	1.06×10^{-2}	5.82×10^{-5}
	20	192.30	18.78	0.9937	1.22×10^{-2}	7.64×10^{-5}
	25	191.61	18.72	0.9952	9.30×10^{-3}	4.44×10^{-5}
	30	186.34	18.13	0.9940	1.17×10^{-2}	6.99×10^{-5}
Šatava-Šesták	5	174.99	16.89	0.9907	1.81×10^{-2}	1.68×10^{-4}
	10	183.31	17.83	0.9926	1.44×10^{-2}	1.07×10^{-4}
	15	189.18	18.49	0.9945	1.06×10^{-2}	5.82×10^{-5}
	20	189.75	18.54	0.9937	1.22×10^{-2}	7.64×10^{-5}
	25	189.09	18.48	0.9952	9.30×10^{-3}	4.44×10^{-5}
	30	184.12	17.92	0.9940	1.17×10^{-2}	6.99×10^{-5}
Agrawal	5	176.11	17.01	0.9898	9.61×10^{-2}	9.78×10^{-4}
	10	184.74	17.98	0.9919	7.67×10^{-2}	6.21×10^{-4}
	15	190.86	18.67	0.9940	5.66×10^{-1}	3.37×10^{-4}
	20	191.40	18.71	0.9932	6.48×10^{-2}	4.43×10^{-4}
	25	190.68	18.65	0.9948	4.95×10^{-2}	2.58×10^{-4}
	30	185.41	18.06	0.9934	6.20×10^{-2}	4.07×10^{-4}
General integral	5	174.73	15.57	0.9897	9.57×10^{-2}	9.85×10^{-4}
	10	183.52	16.53	0.9918	7.63×10^{-2}	6.24×10^{-4}
	15	189.72	17.21	0.9940	5.63×10^{-2}	3.38×10^{-4}
	20	190.33	17.26	0.9931	6.45×10^{-2}	4.44×10^{-4}
	25	189.64	17.21	0.9948	4.92×10^{-2}	2.58×10^{-4}
	30	184.43	16.64	0.9934	6.17×10^{-2}	4.07×10^{-4}
Universal integral	5	176.11	17.02	0.9898	9.61×10^{-2}	9.78×10^{-4}

	10	184.74	17.98	0.9919	7.67×10^{-2}	6.21×10^{-4}
	15	190.86	18.67	0.9940	5.66×10^{-2}	3.37×10^{-4}
	20	191.40	18.71	0.9932	6.48×10^{-2}	4.43×10^{-4}
	25	190.68	18.65	0.9948	4.95×10^{-2}	2.58×10^{-4}
	30	185.41	18.06	0.9934	6.20×10^{-2}	4.07×10^{-4}
Mean		186.18	17.87			
Flynn-Wall-Ozawa		178.36(E_{eo})		0.999		
		185.90(E_{po})		0.9998		
Kissinger		187.43(E_K)	18.47	0.9998		
Mean(E_{eo}, E_{po}, E_K)		183.90				

Note: E with the subscript of eo and po is the apparent activation energy obtained from the onset temperature (T_e) and the peak temperature (T_p) by Ozawa's method, E with the subscript of K is the apparent activation energy obtained from the peak temperature (T_p) by Kissinger's method.

TableS4 Calculated values of kinetic parameters of decomposition reaction for NC.

Method	$\beta/ ^\circ\text{C min}^{-1}$	$E_a/\text{kJ mol}^{-1}$	$\log(A/\text{s}^{-1})$	r	S	d
MacCallum-Tanner	5	207.98	20.55	0.9983	4.45×10^{-4}	7.50×10^{-7}
	10	205.40	20.25	0.9984	4.11×10^{-4}	6.38×10^{-7}
	15	209.33	20.68	0.9988	3.25×10^{-4}	3.98×10^{-7}
	20	209.34	20.67	0.9987	3.49×10^{-4}	4.61×10^{-7}
	25	211.75	20.91	0.9990	2.56×10^{-4}	2.48×10^{-7}
	30	210.10	20.76	0.9982	4.69×10^{-4}	8.30×10^{-7}
Šatava-Šesták	5	204.55	20.23	0.9983	4.45×10^{-4}	7.50×10^{-7}
	10	202.12	19.94	0.9984	4.11×10^{-4}	6.38×10^{-7}
	15	205.83	20.35	0.9988	3.25×10^{-4}	3.98×10^{-7}
	20	205.83	20.33	0.9987	3.49×10^{-4}	4.61×10^{-7}
	25	208.11	20.56	0.9990	2.56×10^{-4}	2.48×10^{-7}
	30	206.56	20.42	0.9982	4.69×10^{-4}	8.30×10^{-7}
Agrawal	5	207.20	20.49	0.9982	2.37×10^{-3}	4.30×10^{-6}
	10	204.54	20.18	0.9983	2.19×10^{-3}	3.67×10^{-6}
	15	208.37	20.60	0.9987	1.73×10^{-3}	2.29×10^{-6}
	20	208.33	20.58	0.9986	1.86×10^{-3}	2.65×10^{-6}
	25	210.68	20.81	0.9990	1.36×10^{-3}	4.43×10^{-6}
	30	209.03	20.66	0.9981	2.49×10^{-3}	4.77×10^{-6}
General integral	5	205.81	18.98	0.9985	2.36×10^{-3}	4.33×10^{-6}
	10	203.30	18.69	0.9983	2.18×10^{-3}	3.69×10^{-6}
	15	207.22	19.10	0.9987	1.72×10^{-3}	2.30×10^{-6}

Universal integral	20	207.24	19.09	0.9986	1.85×10^{-3}	2.66×10^{-6}
	25	209.64	19.33	0.9989	1.36×10^{-3}	4.43×10^{-6}
	30	208.02	19.18	0.9981	2.48×10^{-3}	4.79×10^{-6}
	5	207.20	20.49	0.9982	2.37×10^{-3}	4.30×10^{-6}
	10	204.54	20.19	0.9983	2.19×10^{-3}	3.67×10^{-6}
	15	208.37	20.60	0.9987	1.73×10^{-3}	2.29×10^{-6}
	20	208.33	20.58	0.9986	1.86×10^{-3}	2.65×10^{-6}
	25	210.68	20.82	0.9990	1.36×10^{-3}	4.43×10^{-6}
	30	209.03	20.66	0.9981	2.49×10^{-3}	4.77×10^{-6}
Mean		207.48	20.22			
Flynn-Wall-Ozawa		185.68(E_{eo})		0.9998		
		197.56(E_{po})		0.9979		
Kissinger		199.68(E_K)	19.82	0.9977		
Mean(E_{eo}, E_{po}, E_K)		194.31				

Note: E with the subscript of eo and po is the apparent activation energy obtained from the onset temperature (T_e) and the peak temperature (T_p) by Ozawa's method, E with the subscript of K is the apparent activation energy obtained from the peak temperature (T_p) by Kissinger's method.

TableS5 The values of apparent activation energy (E_a , kJ/mol) of thermal decomposition for NC-Al/Fe₂O₃

NC		NC-Al/Fe ₂ O ₃ (r)		NC-Al/Fe ₂ O ₃ (p)		NC-Al/Fe ₂ O ₃ (o)	
α	$E_{(NL-INT-SY3)}$	α	$E_{(NL-INT-SY3)}$	α	$E_{(NL-INT-SY3)}$	α	$E_{(NL-INT-SY3)}$
0.100	196.22	0.175	193.33	0.100	183.25	0.075	187.12
0.125	196.18	0.200	193.49	0.125	183.55	0.100	186.47
0.150	195.94	0.225	193.70	0.150	183.85	0.125	185.98
0.175	195.66	0.250	193.76	0.175	184.26	0.150	185.56
0.200	195.42	0.275	193.79	0.200	184.66	0.175	185.41
0.225	195.43	0.300	193.80	0.225	185.07	0.200	185.37
0.250	195.43	0.325	193.79	0.250	185.55	0.225	185.40
0.275	195.44	0.350	193.84	0.275	186.06	0.250	185.54
0.300	195.43	0.375	193.88	0.300	186.56	0.275	185.78
0.325	195.51	0.400	193.96	0.325	187.16	0.300	186.08
0.350	195.68	0.425	194.07	0.350	187.73	0.325	186.34
0.375	195.82	0.450	194.22	0.375	188.38	0.350	186.65
0.400	196.02	0.475	194.42	0.400	189.03	0.375	186.94
0.425	196.19	0.500	194.70	0.425	189.67	0.400	187.26
0.450	196.36	0.525	195.01	0.450	190.32	0.425	187.63
0.475	196.53	0.550	195.48	0.475	191.05	0.450	189.34
0.500	196.78	0.575	196.06	0.500	191.79	0.475	188.39
0.525	197.11	0.600	196.73	0.525	192.57	0.500	188.87
0.550	197.51	0.625	197.53	0.550	193.42	0.525	189.45
0.575	198.02	0.650	198.56	0.575	194.31	0.550	190.13
0.600	198.56	0.675	199.84	0.600	195.29	0.575	190.92
0.625	199.21			0.625	196.37	0.600	191.87
0.650	200.05			0.650	197.56	0.625	192.99
0.675	200.98			0.675	198.94	0.650	194.38
0.700	202.06			0.700	200.42	0.675	195.97
0.725	203.49			0.725	202.17	0.700	197.91
0.750	205.16			0.750	204.11	0.725	200.16
0.775	207.46			0.775	206.44	0.750	202.82
0.800	210.32			0.800	209.06	0.775	206.02
						0.800	209.96
Mean(E_N)	198.27		194.95		192.02		190.76
Mean(E_a)	207.48		182.53		191.75		186.18

Note: E with the subscript of a is the apparent activation energy obtained by logical choice method, E with the subscript of NL-INT-SY3 is the apparent activation energy obtained by an integral isoconversional non-linear (NL-INT) method.