Electronic Supplementary Information

Prototypical iron(II) complex with 4-amino-1,2,4-triazole reinvestigated: an unexpected impact of water on spin transition

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Table of contents

Fig. S1 Quartz ampoules for magnetic measurements (left) and crucibles for DSC (right). Ampoules: sealed ampoule with the sample and a non-sealed free ampoule are shown. Crucibles: sealed crucible and an open crucible with the sample.
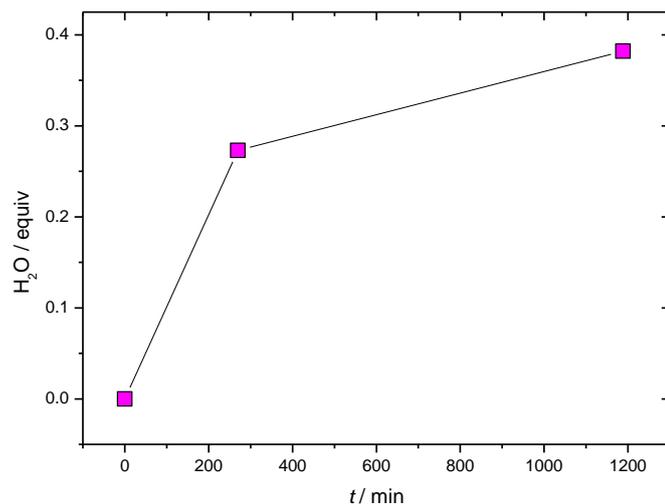
Fig. S2 Water sorption curve for $Fe(ATrz)_3(NO_3)_2 \cdot H_2O$ (the sample **3**).
The sample **3** was placed into a quartz ampoule and exposed to water vapor for 20 h (mass increase 1.5 %, 0.37 equiv. of H_2O). Increase in the mass of this sample was monitored by weighing the ampoule with the sample.
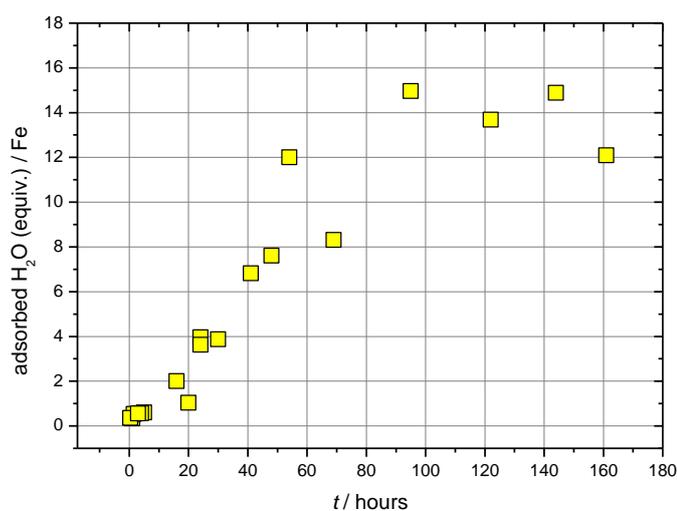
Fig. S3 Rate of water adsorption for aged $Fe(ATrz)_3(NO_3)_2 \cdot 0.5H_2O$.
The samples were placed into DSC crucibles and exposed to water vapor. Every point corresponds to a separate sample. Increase in the mass of the samples was monitored by weighing.
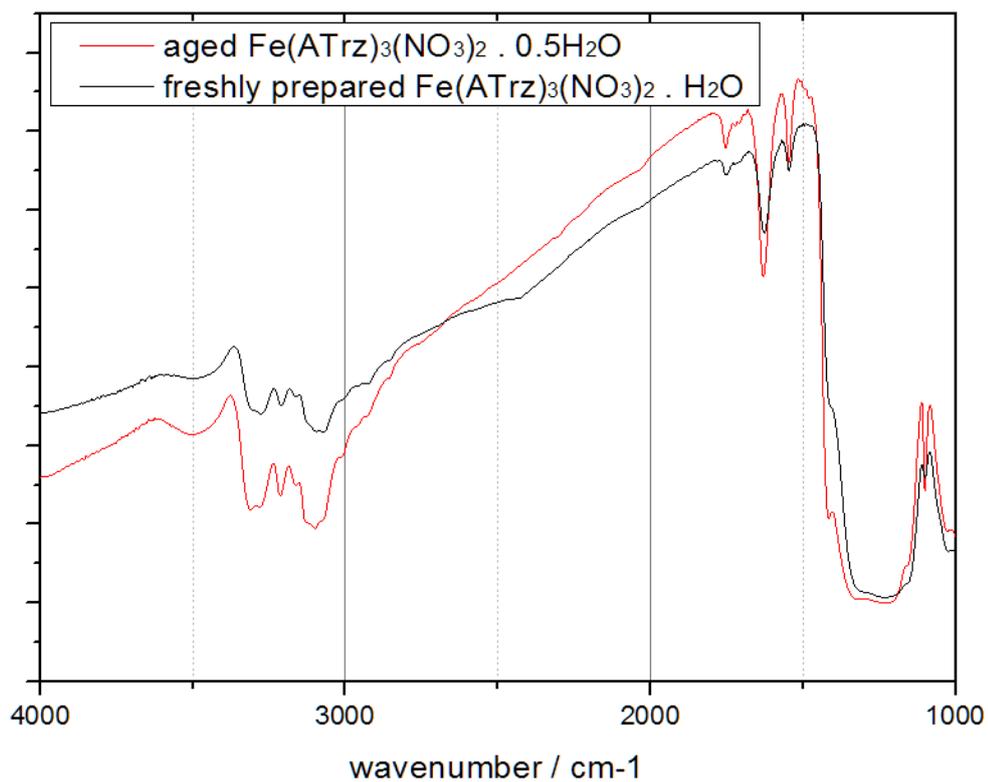
Fig. S4 IR spectra of freshly prepared $Fe(ATrz)_3(NO_3)_2 \cdot H_2O$ and aged $Fe(ATrz)_3(NO_3)_2 \cdot 0.5H_2O$ in fluorinated oil.
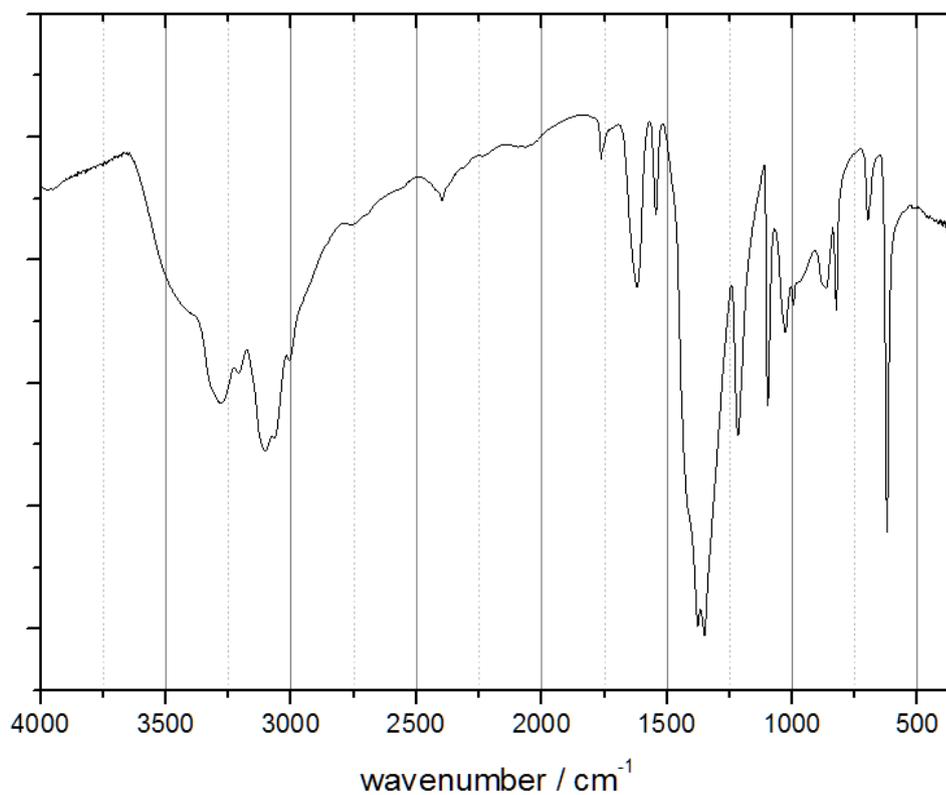
Fig. S5 IR spectrum of freshly prepared $Fe(ATrz)_3(NO_3)_2 \cdot H_2O$ in KBr.
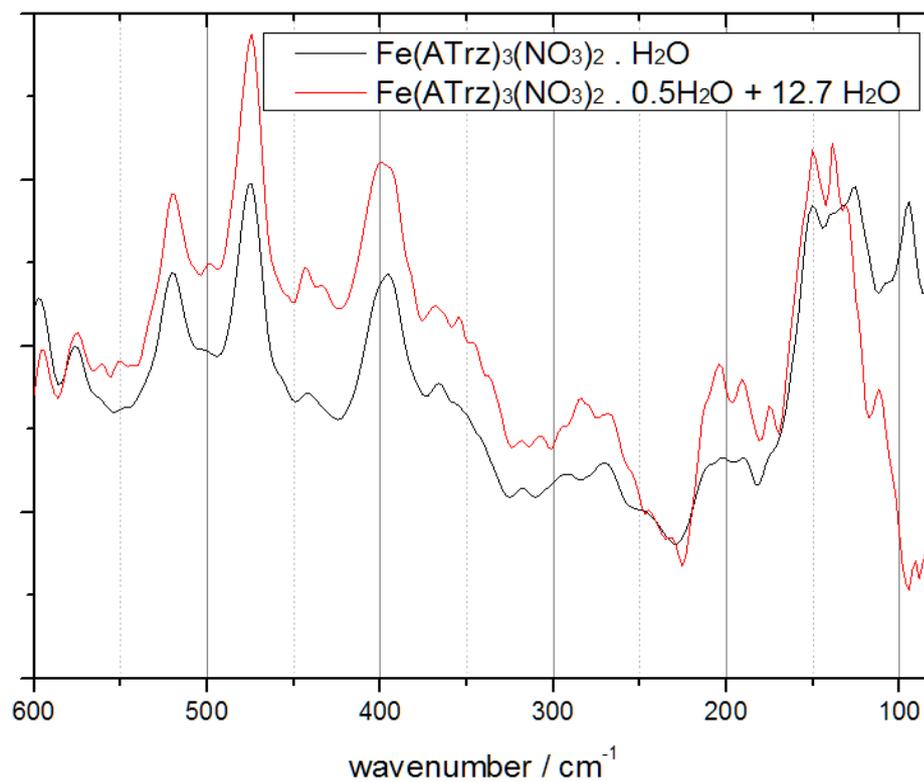
Fig. S6 Far IR spectra (in polyethylene) of freshly prepared $Fe(ATrz)_3(NO_3)_2 \cdot H_2O$ and aged $Fe(ATrz)_3(NO_3)_2 \cdot 0.5H_2O$ after adsorbing 12.7 equiv. of H_2O.
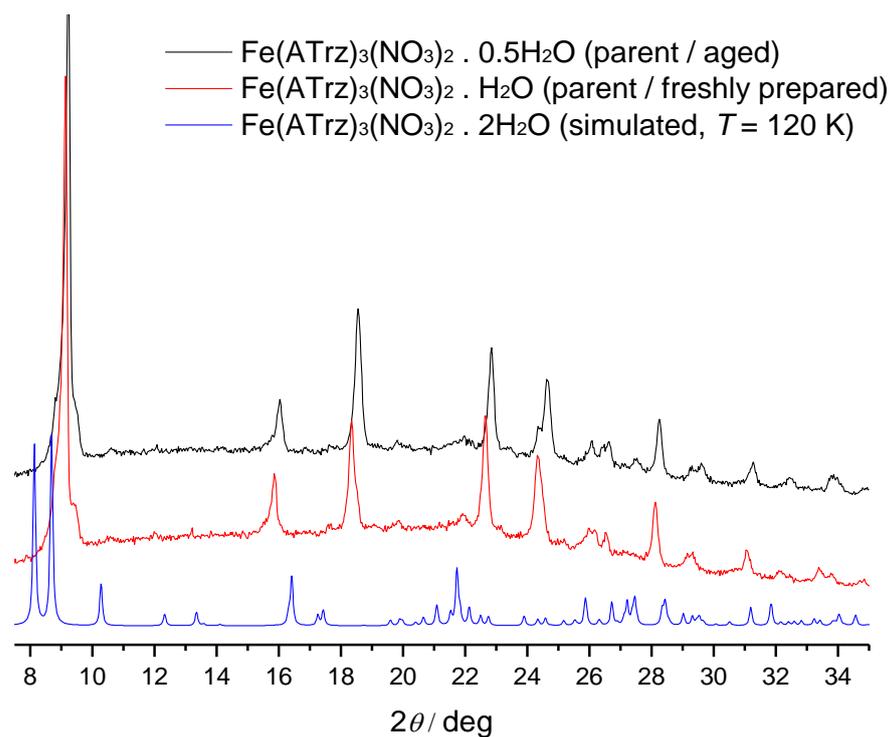
Fig. S7 X-ray powder patterns of freshly prepared $Fe(ATrz)_3(NO_3)_2 \cdot H_2O$ and aged $Fe(ATrz)_3(NO_3)_2 \cdot 0.5H_2O$ and simulated pattern of $Fe(ATrz)_3(NO_3)_2 \cdot 2H_2O$.
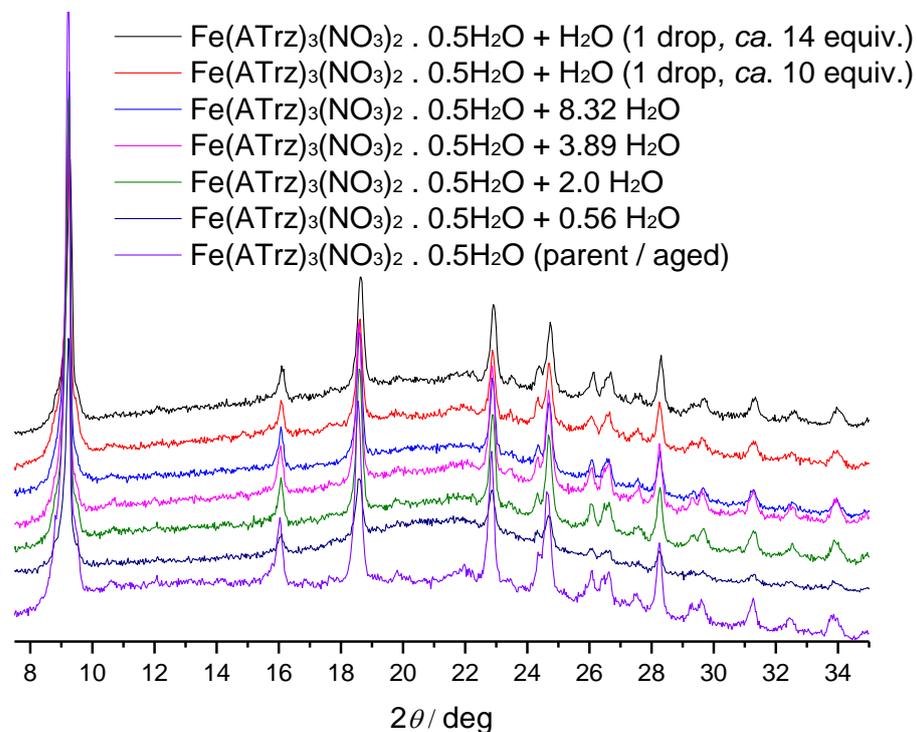
Fig. S8 X-ray powder patterns of aged $Fe(ATrz)_3(NO_3)_2 \cdot 0.5H_2O$ after adsorption or addition of various amount of H_2O.
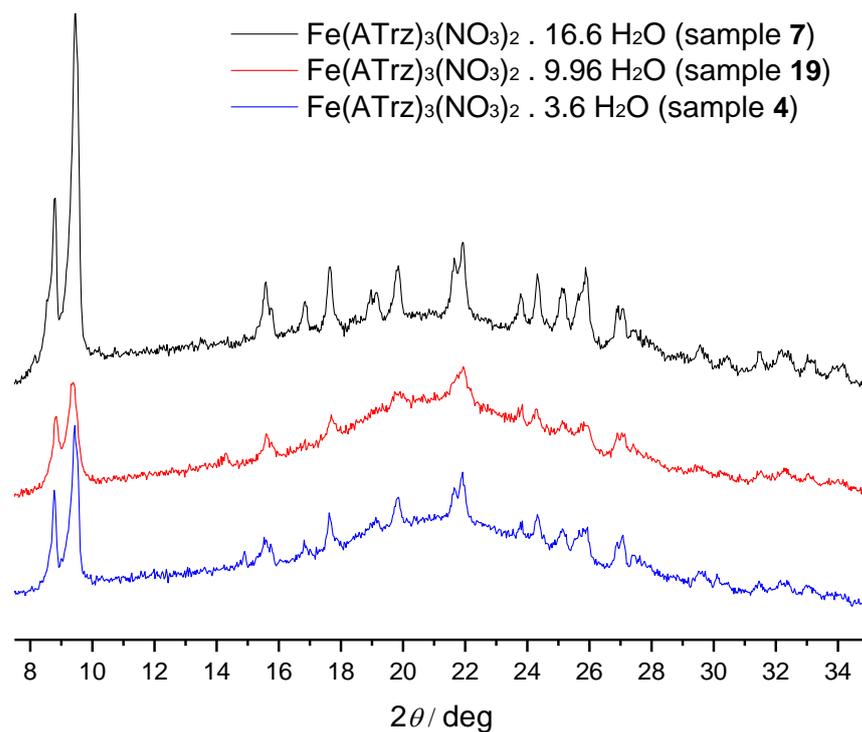
Fig. S9 X-ray powder patterns of Fe(ATrz)$_3$(NO$_3$)$_2$·nH$_2$O (n = 3.6 – 16.6).
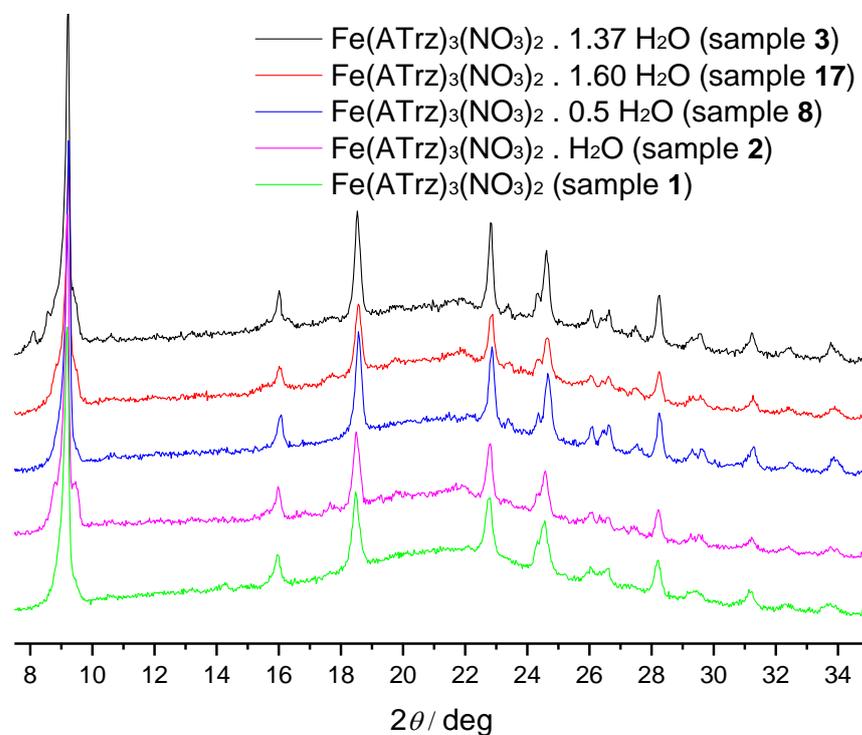
Fig. S10 X-ray powder patterns of Fe(ATrz)$_3$(NO$_3$)$_2$·nH$_2$O (n = 0.5 – 1.60) and Fe(ATrz)$_3$(NO$_3$)$_2$.
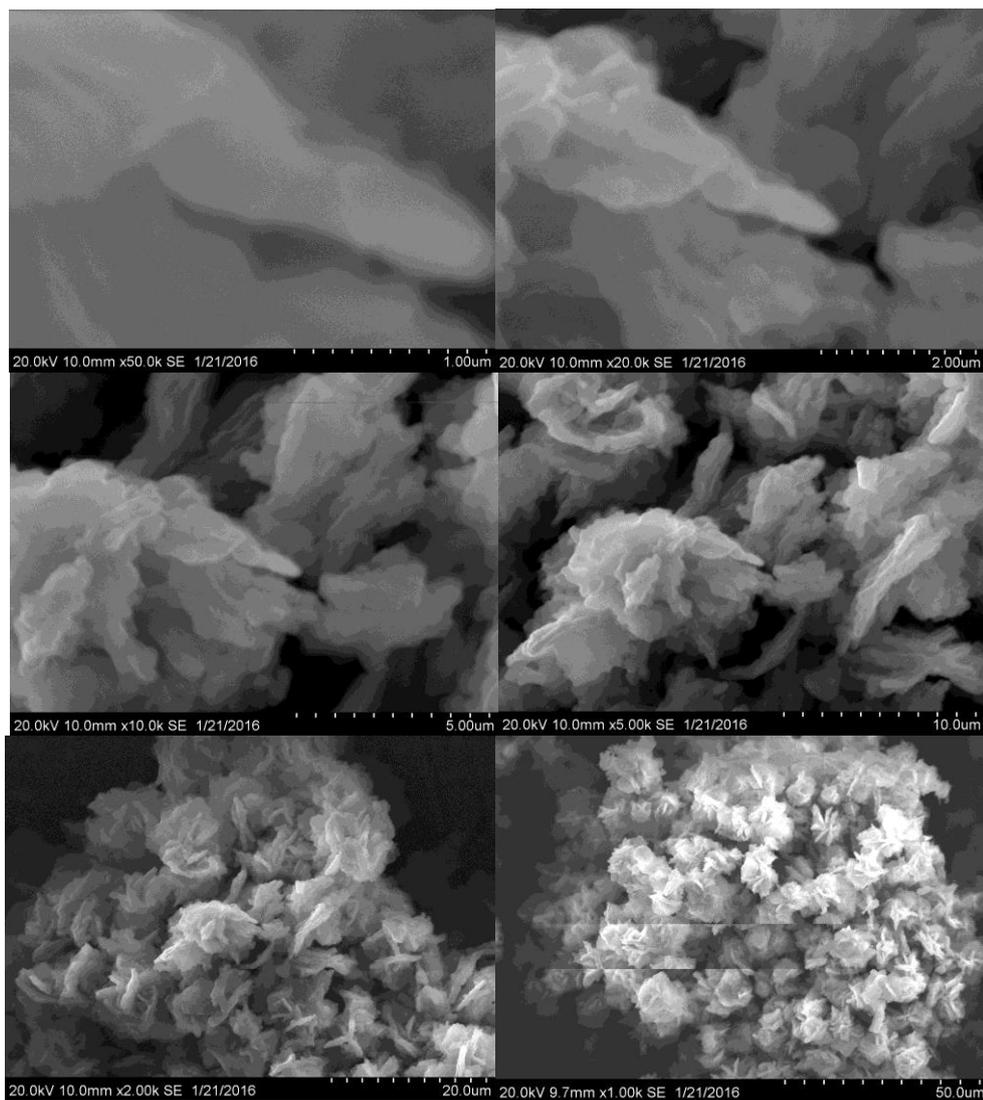
Fig. S11 SEM images of the phase Fe(ATrz)$_3$(NO$_3$)$_2\cdot$H$_2$O.
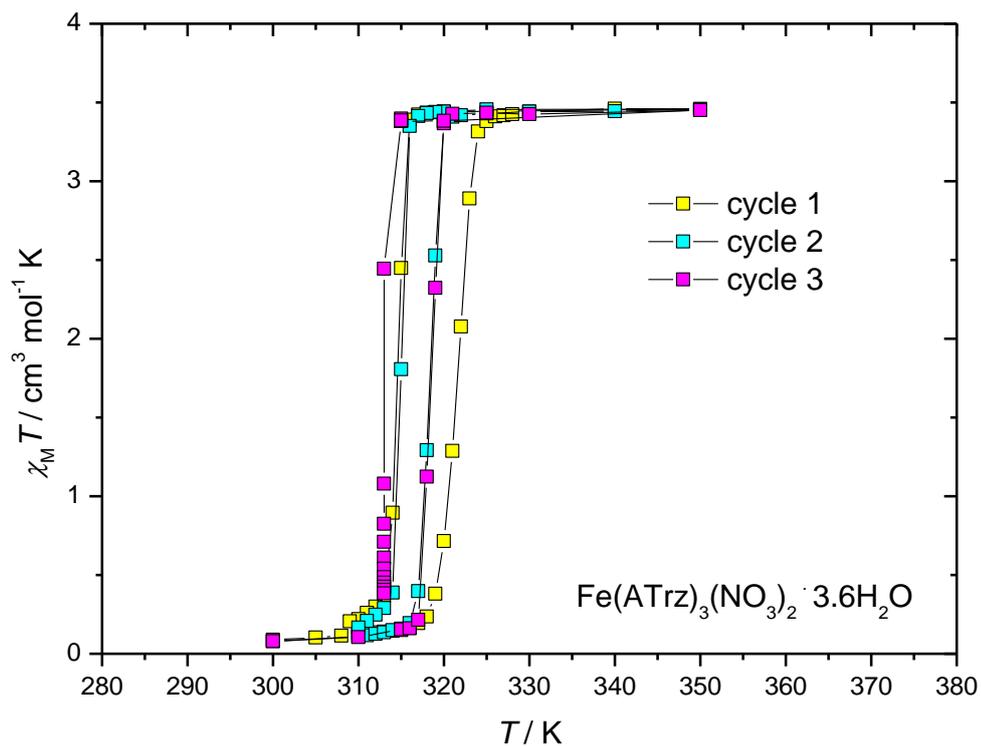
Fig. S12 Thermal cycles for Fe(ATrz)₃(NO₃)₂·3.6H₂O (the sample **4**).
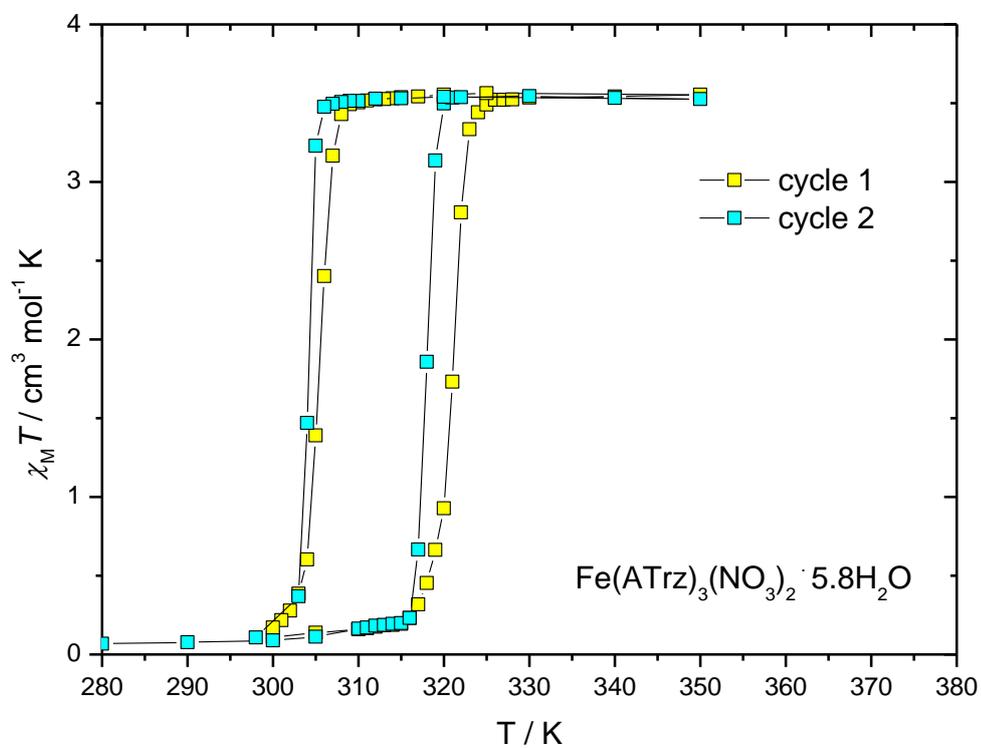
Fig. S13 Thermal cycles for Fe(ATrz)₃(NO₃)₂·5.8H₂O (the sample **5**).
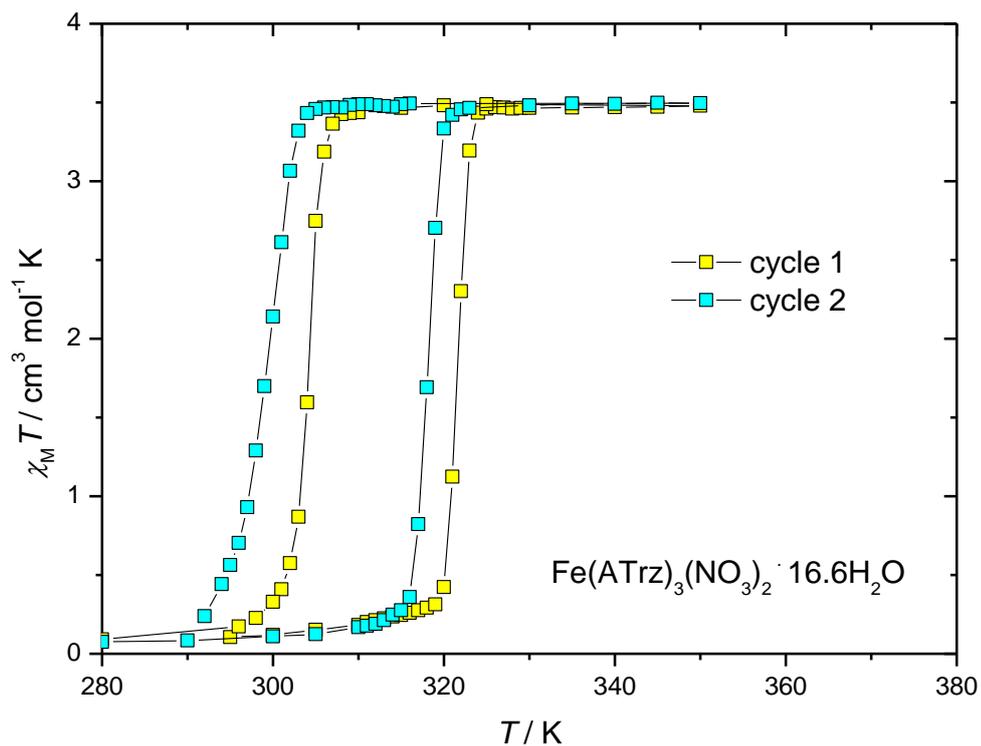
Fig. S14 Thermal cycles for Fe(ATrz)$_3$(NO$_3$)$_2$·16.6H$_2$O (the sample **7**).
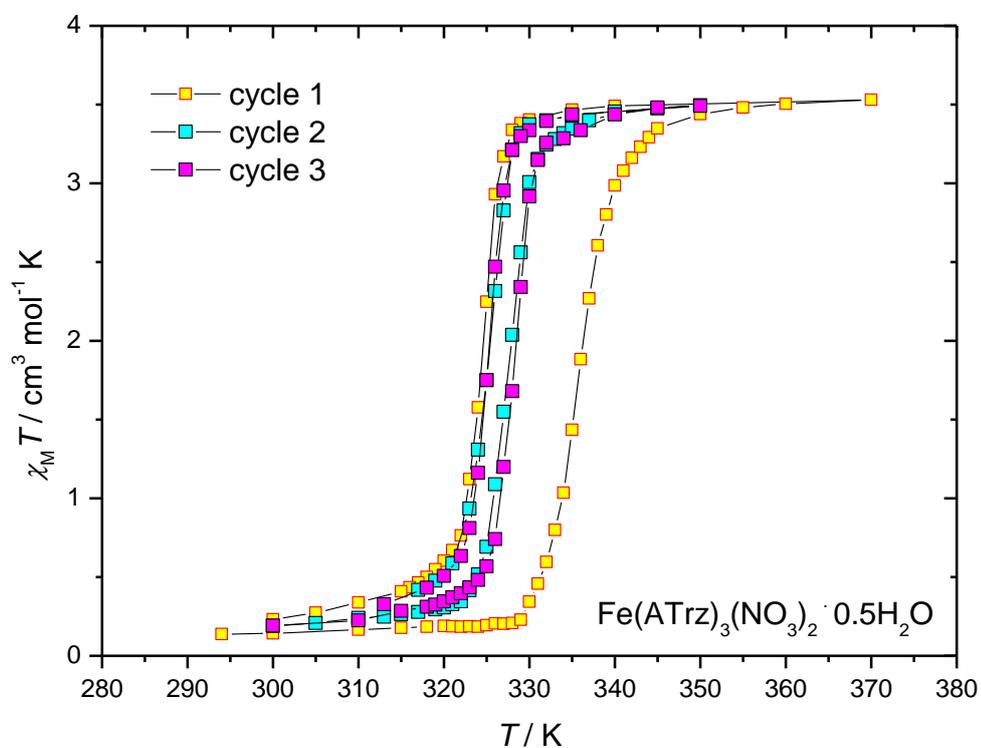
Fig. S15 Thermal cycles for Fe(ATrz)$_3$(NO$_3$)$_2$·0.5H$_2$O (the sample **8**).

Kinetic curves: fitting

Kinetics curves are shown in Figs. S16–S19 and results of fitting are collected in Table S1.

Fitting of exponential curves has been done in the frame of mono-, bi- or tri-exponential approximations using following equations.

(1) Monoexponential approximation

(1a) Monoexponential decay

$$\chi_M T = [(\chi_M T)_{max} - (\chi_M T)_{min}]e^{\left(-\frac{t}{\tau_1}\right)} + (\chi_M T)_{min}$$
$$= [(\chi_M T)_{max} - (\chi_M T)_{min}]e^{(-k_1 t)} + (\chi_M T)_{min},$$

(1b) Monoexponential decelerating growth

$$\chi_M T = [(\chi_M T)_{min} - (\chi_M T)_{max}]e^{\left(-\frac{t}{\tau_1}\right)} + (\chi_M T)_{max}$$
$$= [(\chi_M T)_{max} - (\chi_M T)_{min}]e^{(-k_1 t)} + (\chi_M T)_{max}$$

These equations can be rewritten as

$$\chi_M T \equiv A_1 e^{(-k_1 t)} + y_0,$$

with

$(\chi_M T)_{max} = A_1 + y_0,$
$(\chi_M T)_{min} = y_0$
for exponential decay,
and with
$(\chi_M T)_{min} = A_1 + y_0, (A_1 < 0),$
$(\chi_M T)_{max} = y_0$
for exponential decelerating growth.

(2) Biexponential approximation (biexponential decay)

$$\chi_M T = A\left\{[(\chi_M T)_{max} - (\chi_M T)_{min}]e^{\left(-\frac{t}{\tau_1}\right)} + (\chi_M T)_{min}\right\} + (1 - A)\left\{[(\chi_M T)_{max} - \right.$$

$$(\chi_M T)_{min}]e^{\left(-\frac{t}{\tau_2}\right)} + (\chi_M T)_{min}\right\} = A\left\{[(\chi_M T)_{max} - (\chi_M T)_{min}]e^{(-k_1 t)} + (\chi_M T)_{min}\right\} +$$

$$(1 - A)\left\{[(\chi_M T)_{max} - (\chi_M T)_{min}]e^{(-k_2 t)} + (\chi_M T)_{min}\right\} \equiv A_1 e^{(-k_1 t)} + A_2 e^{(-k_2 t)} + y_0,$$

$(\chi_M T)_{max} = A_1 + A_2 + y_0,$
$(\chi_M T)_{min} = y_0,$
$$A = \frac{A_1}{A_1 + A_2}.$$

(3) Triexponential approximation (triexponential decay)

$$\chi_M T = A\left\{[(\chi_M T)_{max} - (\chi_M T)_{min}]e^{\left(-\frac{t}{\tau_1}\right)} + (\chi_M T)_{min}\right\}$$

$$+ B\left\{[(\chi_M T)_{max} - (\chi_M T)_{min}]e^{\left(-\frac{t}{\tau_2}\right)} + (\chi_M T)_{min}\right\}$$

$$+ (1 - A - B)\left\{[(\chi_M T)_{max} - (\chi_M T)_{min}]e^{\left(-\frac{t}{\tau_3}\right)} + (\chi_M T)_{min}\right\}$$

$$= A\{[(\chi_M T)_{max} - (\chi_M T)_{min}]e^{(-k_1 t)} + (\chi_M T)_{min}\}$$

$$+ B\{[(\chi_M T)_{max} - (\chi_M T)_{min}]e^{(-k_2 t)} + (\chi_M T)_{min}\}$$

$$+ (1 - A - B)\left\{[(\chi_M T)_{max} - (\chi_M T)_{min}]e^{\left(-\frac{t}{\tau_3}\right)} + (\chi_M T)_{min}\right\}$$

$$\equiv A_1 e^{(-k_1 t)} + A_2 e^{(-k_2 t)} + A_3 e^{(-k_3 t)} + y_0$$

$$(\chi_M T)_{max} = A_1 + A_2 + A_3 + y_0,$$
$$(\chi_M T)_{min} = y_0,$$
$$A = \frac{A_1}{A_1 + A_2 + A_3},$$
$$B = \frac{A_2}{A_1 + A_2 + A_3},$$

where k_i (rate constants) or τ_i (lifetimes for ith exponent, $\tau_i = 1/k_i$), A_i (preexponents) and y_0 are fitting parameters, $(\chi_M T)_{max}$ and $(\chi_M T)_{min}$ are the highest and the lowest $\chi_M T$ values for a kinetic curve and A and B are the population ratios of the states responsible for the decay with the rate constants k_1 and k_2.

(4) For exponential decay yield for ith exponent, R_i, can be calculated as

$$R_i = \frac{\int_0^\infty A_i e^{-\frac{t}{\tau_i}} dt}{\sum_{i=1}^m \int_0^\infty A_i e^{-\frac{t}{\tau_i}} dt} = \frac{A_i \tau_i}{\sum_{i=1}^m A_i \tau_i},$$

where m is the number of exponents.

(5) Decay with a shape intermediate between sigmoidal and exponential decelerating

Relaxation curves having both exponential decelerating and sigmoidal character can be fitted using the equation combining both sigmoidal and exponential decay components. We combined here the Johnson-Mehl-Avrami-Kolmogorov equation[S1] and the equation describing monoexponential decay:

$$\chi_M T = A\{[(\chi_M T)_{max} - (\chi_M T)_{min}]e^{(-(k_1 t)^n)} + (\chi_M T)_{min}\} + (1 - A)\{[(\chi_M T)_{max} - (\chi_M T)_{min}]e^{(-k_2 t)} + (\chi_M T)_{min}\} \equiv A_1 e^{(-(k_1 t)^n)} + A_2 e^{(-k_2 t)} + y_0,$$

with

$$(\chi_M T)_{max} = A_1 + A_2 + y_0,$$

$$(\chi_M T)_{min} = y_0,$$

$$A = \frac{A_1}{A_1 + A_2},$$

where k_i (rate constants), n (Avrami exponent), A_i (preexponents) and y_0 are fitting parameters, $(\chi_M T)_{max}$ and $(\chi_M T)_{min}$ are the highest and the lowest $\chi_M T$ values for a kinetic curve and A is the population ratio of the state responsible for the decay with the rate constant k_1.

S1 W. A. Johnson and R. F. Mehl, *Trans. Am. Inst. Min. Eng.*, 1939, **135**, 416–458; M. Avrami, *J. Chem. Phys.*, 1939, **7**, 1103–1112; A. N. Kolmogorov, *Bull. Acad. Sci. USSR, Phys. Ser.*, 1937, **1**, 355–359.
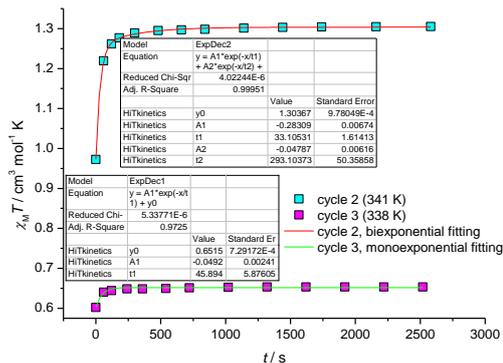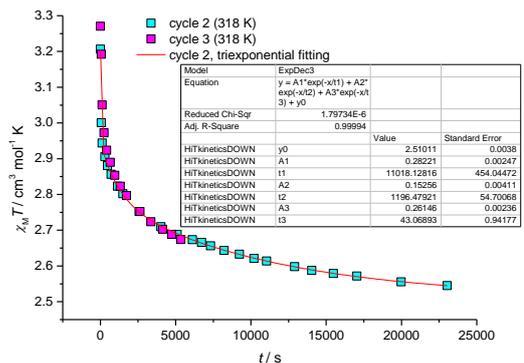
Fig. S16 Kinetic curves for the sample **1**.
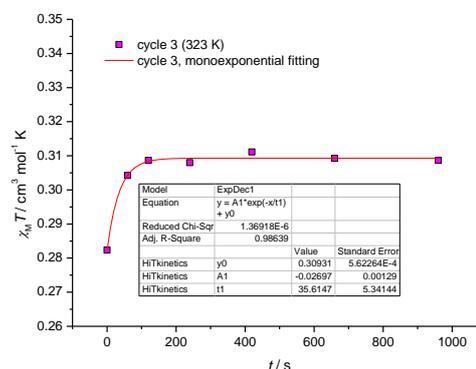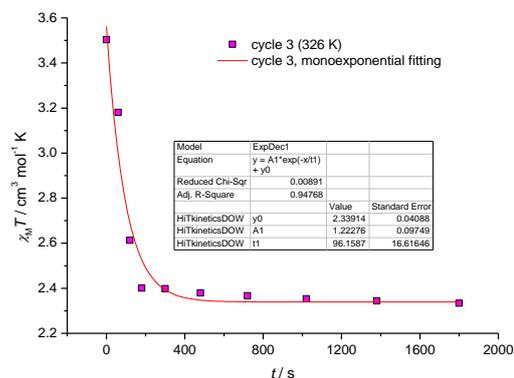
Fig. S17 Kinetic curves for the sample **2**.
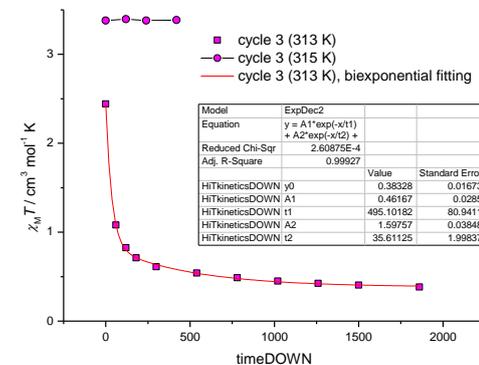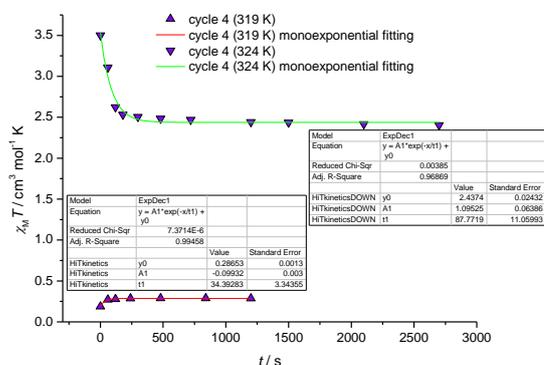
Fig. S18 Kinetic curves for the sample **3** (left) and sample **4** (right, annealing at 315 K did not reveal any lowering of the magnetic moment, but after fast cooling to 313 K we observed very fast exponential decay).
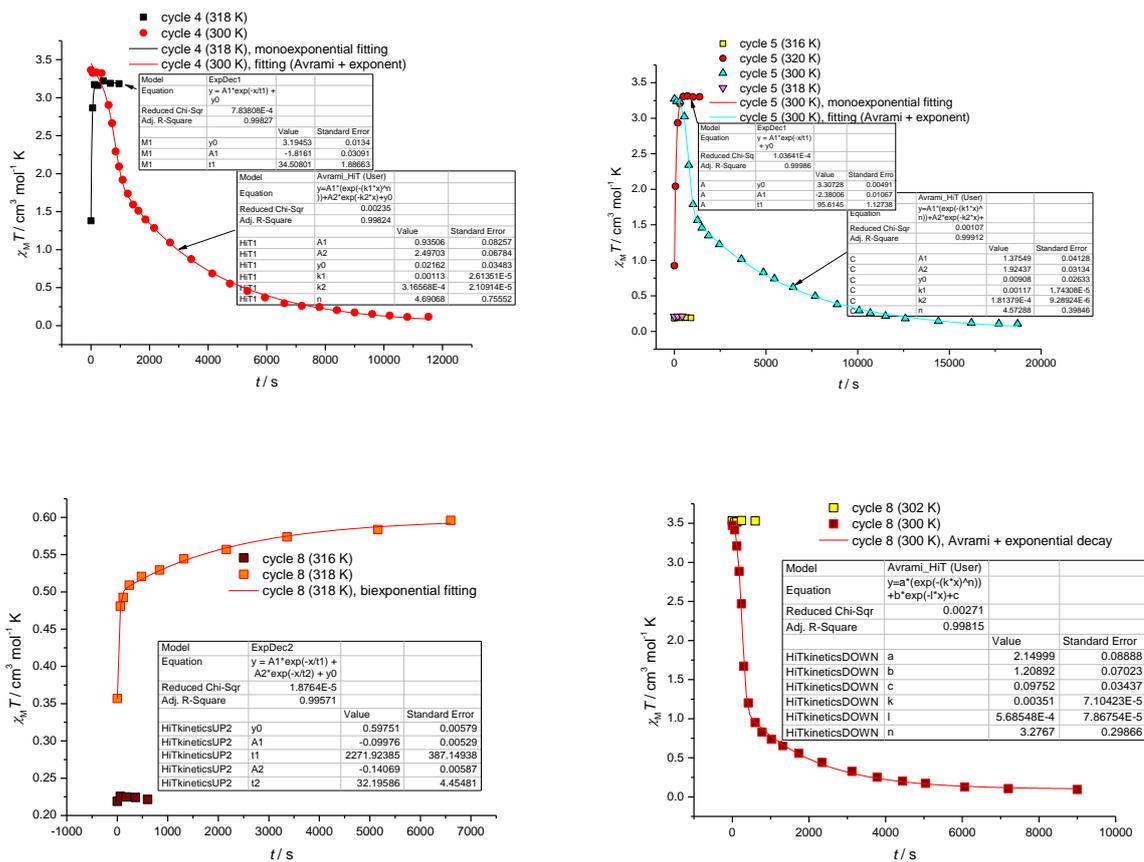
Fig. S19 Kinetic curves for the samples **6** (top) and **9** (bottom).
Isothermal annealing of the sample **9** in the 8th thermal cycle at 302 K (Fig S19, bottom, right) did not reveal any decrease in the magnetic moment values for 10 min.

Table S1. Kinetic parameters y_0 (cm³mol⁻¹K), A_i (cm³mol⁻¹K), τ_i (s), k_i (s⁻¹), n, A, B, $(\chi_M T)_{max}$ (cm³mol⁻¹K) and $(\chi_M T)_{min}$ (cm³mol⁻¹K) for the LS → HS and the HS → LS isothermal transformations. Kinetic curves are shown in Figs. S16 – S19.

Sample	Cycle	y_0	A_1	τ_1	k_1	A_2	τ_2	k_2	A_3	τ_3	k_3	n	A	B	$(\chi_M T)_{max}$	$(\chi_M T)_{min}$
1	cycle 2 (341 K)	1.304	-0.283	3.3×10^1	3.0×10^{-2}	-0.047	2.9×10^2	3.4×10^{-3}					0.86		1.30	1.02
	cycle 2 (318 K)	2.51	0.282	1.1×10^4	9.1×10^{-5}	0.15	1.2×10^3	8.3×10^{-4}	0.261	4.31×10^1	0.0232		0.65	0.22	3.20	2.51
	cycle 3 (338 K)	0.6515	-0.049	4.6×10^1	2.2×10^{-2}										0.65	0.60
2	cycle 3 (326 K)	2.34	1.22	9.6×10^1	1.0×10^{-2}										3.56	2.34
	cycle 3 (323 K)	0.3093	-0.0217	3.6×10^1	2.8×10^{-2}										0.31	0.29
3	cycle 4 (324 K)	0.287	-0.0993	3.4×10^1	2.9×10^{-2}										0.29	0.19
	cycle 4 (319 K)	2.44	1.1	8.8×10^1	1.1×10^{-2}										3.54	2.44
4	cycle 3 (313 K)	0.383	0.46	5.0×10^2	2.0×10^{-3}	1.60	3.6×10^1	2.8×10^{-2}					0.22		2.44	0.383
6	cycle 4 (318 K)	3.19	-1.82	3.5×10^1	2.9×10^{-2}										3.19	1.37
	cycle 4 (300 K)	0.02	0.94	8.85×10^2	1.13×10^{-3}	2.5	2.92×10^3	3.42×10^{-4}				4.7	0.27		3.46	0.02
	cycle 5 (320 K)	3.307	-2.8	9.6×10^1	1.0×10^{-2}										3.31	0.51
	cycle 5 (300 K)	0.009	1.38	8.55×10^2	1.17×10^{-3}	1.92	5.52×10^3	1.81×10^{-4}				4.6	0.42		3.31	0.009
9	cycle 8 (318 K)	0.598	-0.0998	2.3×10^3	4.4×10^{-4}	-0.141	3.2×10^1	3.1×10^{-2}					0.41		0.60	0.36
	cycle 8 (300 K)	0.098	2.15	2.9×10^2	3.5×10^{-3}	1.21	1.8×10^3	5.6×10^{-4}				3.3	0.64		3.46	0.098
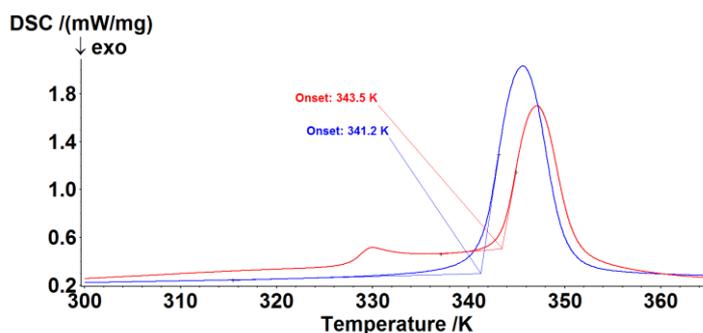
Fig. S20 The sample **10**: comparison of the first cycle (red line) and the tenth cycle (blue line).
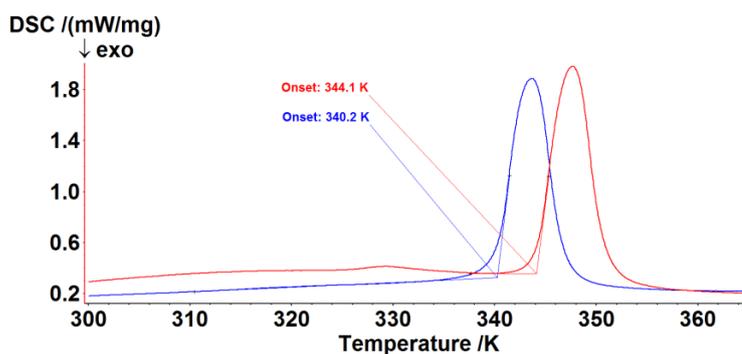
Fig. S21 The sample **11**: comparison of the first cycle (red line) and the sixteenth cycle (blue line).
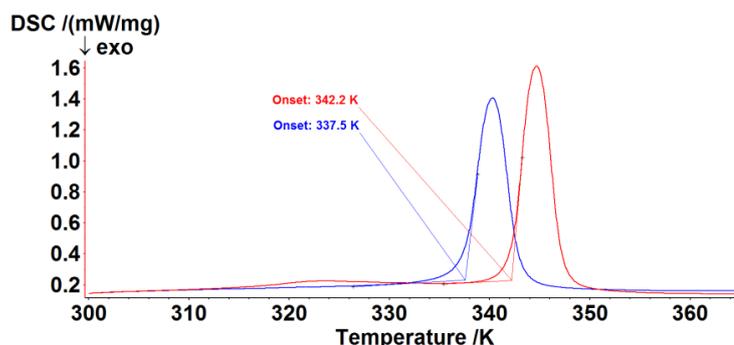
Fig. S22 The sample **12**: comparison of the first cycle (red line) and the ninth cycle (blue line).
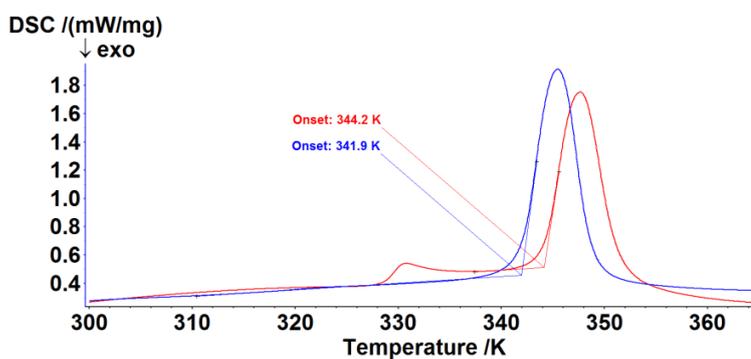
Fig. S23 The sample **13**: comparison of the first cycle (red line) and the forth cycle (blue line).

Table S2. Magnetochemical data for the samples **1** – **9**.

Sample	Conditions / formula	Cycle	Day	$T_c\uparrow$, K	$T_c\downarrow$, K	ΔT
1	Vacuum, $Fe(ATrz)_3(NO_3)_2$	1	1st	345	317	28
		2	1st	(341 kin.), 345	(318 kin.)	
		3	3rd	(338 kin.), 345	(318 kin), 315	30
		4	3rd	343	314	29
2	Sealed ampoule, $Fe(ATrz)_3(NO_3)_2 \cdot H_2O$	1	1st	326	325	1
		2	1st	327	324	3
		3	1st	(323 kin.), 327	(326 kin.), 324	3
		4	7th	328	326	2
		5	363rd	328	325	3
3	Sealed ampoule, $Fe(ATrz)_3(NO_3)_2 \cdot 1.37H_2O$	1	1st	319/326	317/322	2/4
		2	1st	320/327	317/324	3/3
		3	1st	320/327	317/324	3/3
		4	1st	(319 kin.), 320/327	(324 kin.)	
		5	15th	321/328	318/324	3/4
		6	375th	321/329	316/324	5/5
4	Sealed ampoule, $Fe(ATrz)_3(NO_3)_2 \cdot 3.6H_2O$	1	1st	322	315	7
		2	1st	319	315	4
		3	1st	319	(313 kin.)	
5	Sealed ampoule, $Fe(ATrz)_3(NO_3)_2 \cdot 5.8H_2O$	1	1st	321	305	16
		2	1st	318	304	14
6	Sealed ampoule, $Fe(ATrz)_3(NO_3)_2 \cdot 15H_2O$	1	1st	321	302	19
		2	1st	319	301	18
		3	1st	319	301	18
		4	1st	(318 kin.)	(300 kin.)	
		5	15th	(316, 318, 320 kin.)	(300 kin.)	
		6	15th	320	301	19
7	Sealed ampoule, $Fe(ATrz)_3(NO_3)_2 \cdot 16.6H_2O$	1	1st	321	304	17
		2	1st	318	300	18
8	Sealed ampoule, $Fe(ATrz)_3(NO_3)_2 \cdot 0.5H_2O$	1	1st	335	325	10
		2	1st	328	326	2
		3	1st	329	325	4
9	Vacuum, $Fe(ATrz)_3(NO_3)_2$	1	1st	345	316	29
	Sealed ampoule, $Fe(ATrz)_3(NO_3)_2 \cdot 0.5H_2O$	2	2nd	334	324	10
		3	2nd	327	325	2
		4	2nd	327	325	2
	Vacuum, $Fe(ATrz)_3(NO_3)_2$	5	2nd	345	313	32
	Sealed ampoule, $Fe(ATrz)_3(NO_3)_2 \cdot 10.6H_2O$	1	9th	321	303	18
		2	9th	318	302	16
		3	9th	(316, 318 kin.), 320	(302, 300 kin.)	

Temperatures at which isothermal kinetic experiments have been performed are labelled by the abbreviation "kin.".

Table S3. DSC data for the samples **10 – 20**.

Sample	Conditions / formula	Cycle	Day	Heating rate, K/min	$T\uparrow_{onset}$, K	$T\downarrow_{onset}$, K	ΔH, J mol^{-1}	ΔS, J mol^{-1} K^{-1}	CnB model				Fn model		
									n	logK_{cat}	E_a, kJ mol^{-1}	log$A$	n	E_a, kJ mol^{-1}	log$A$
10	Open crucible, Fe(ATrz)$_3$(NO$_3$)$_2$	1	1st	9	343.5		18839	53.9							
		2	3rd	9	343.3		19185	54.7							
		3	3rd	9	342.2		22339	64.3	2.96	-2.39	1312	198.4	2.67	1169	176.7
		4	3rd	9	341.8		22123	63.6	2.79	-0.50	1194	180.5	2.60	1159	175.2
		5	6th	9	343.3		22296	63.8	3.15	0.22	1213	182.6	3.05	1361	205.7
		6	6th	9	341.9		22642	65.3	2.76	0.17	1069	161.4	2.70	1222	184.8
		7	7th	9	341.5		22685	65.5	2.86	0.22	1107	167.4	2.79	1279	193.8
		8	8th	9	342.8		22426	64.3	2.71	0.070	1437	217.1	3.11	1417	214.1
		9	8th	6	341.5		22728	65.5	3.30	-0.28	1311	198.4	2.57	1394	211.2
		10	8th	12	341.5		22512	64.9	3.11	-0.098	1130	171.0	2.88	1137	172.2
11	Open crucible, Fe(ATrz)$_3$(NO$_3$)$_2$	1	1st	9	344.1		22771	65.1	2.77	-4.0	1399	210.4	2.71	1336	200.9
		2	2nd	9	342.6		22123	63.4	2.98	-0.85	1369	206.8	2.43	1214	183.2
		3	2nd	9	341.2		21821	62.8	2.53	-4.0	1234	187.0	2.32	1145	173.5
		4	2nd	9	340.2		21778	62.0	2.41	-1.30	1154	175.2	2.23	1050	159.4
		5	5th	9	343.4		21475	62.2	2.85	-0.40	1230	185.3	2.54	1244	187.3
		6	5th	9	341.1		20870	59.8	2.44	-0.21	1027	155.3	2.20	1015	153.5
		7	5th	9	341.7		22296	64.1	2.73	-0.90	1274	192.8	2.49	1232	186.5
		8	6th	9	341.8		21432	61.5	2.76	-0.39	1198	181.3	2.39	1142	172.7
		9	6th	9	340.0		21043	60.4	2.36	-0.47	1102	167.3	2.24	1031	156.4
		10	6th	9	339.1		21864	62.9	2.72	-0.17	1139	172.9	2.32	1090	165.5
		11	6th	9	339.9		21864	63.1	2.46	0.17	997	151.1	2.32	1090	165.5
		12	6th	9	338.9		21648	62.2	2.76	-0.61	1274	192.9	2.50	1268	192.0
		13	6th	9	340.4		21734	62.8	2.60	-0.91	1206	183.1	2.35	1121	170.2
		14	6th	9	340.2		21864	63.1	2.59	-0.58	1177	178.8	2.49	1133	172.0
		15	7th	9	341.8		21864	62.8	3.07	-0.013	1237	187.3	2.76	1306	197.9
		16	7th	9	340.2		21994	63.4	2.70	-0.54	1246	189.4	2.57	1268	192.9
		17	7th	9	341.2		22123	63.6	3.01	-0.22	1285	195.0	2.71	1298	196.9

12	Open crucible, Fe(ATrz)$_3$(NO$_3$)$_2$	1	1st	6	342.2		22555	64.9	2.57	0.50	1263	190.7	2.75	1819	275.7
		2	1st	6	339.9		22555	65.3	2.51	0.53	1165	177.0	2.66	1678	256.0
		3	1st	6	338.9		22555	65.3	2.68	0.28	1302	198.6	2.52	1549	236.7
		4	1st	6	338.4		21821	63.3	2.64	0.27	1246	190.2	2.33	1401	214.3
		5	3rd	6	340.0		21821	63.1	2.43	0.75	1000	151.5	2.70	1621	247.2
		6	3rd	6	338.9		21907	63.6	2.64	0.40	1253	191.2	2.54	1566	239.5
		7	3rd	6	338.1		21562	62.7	2.69	-0.034	1420	217.3	2.34	1419	217.3
		8	3rd	6	337.4		21259	63.8	2.63	-0.15	1363	208.9	2.21	1290	197.7
		9	3rd	6	337.6		21648	63.0	2.68	0.03	1336	204.7	2.22	1309	200.5
13	Open crucible, Fe(ATrz)$_3$(NO$_3$)$_2$	1	1st	9	344.2	317.1	19488	56.0	2.98	0.13	1087	163.1	3.07	1283	192.9
		2	1st	9	344.6	316.9	19660	56.4	2.42	-0.15	1076	162.1	2.46	1143	172.3
		3	1st	9	343.4	316.1	20525	59.3	2.20	0.22	1003	151.0	2.69	1326	200.0
		4	1st	9	342.0	316.3	20697	59.4	2.54	-0.045	1081	163.2	2.39	1160	175.3
14	Sealed crucible, Fe(ATrz)$_3$(NO$_3$)$_2$·H$_2$O	1	1st	9	328.9		25529	76.4							
		2	1st	9	326.1		22467	67.6							
		3	2nd	9	326.6		22873	69.0							
		4	2nd	9	326.3		22467	66.8							
		5	5th	9	326.4		22152	66.4							
		6	5th	9	326.2		22692	68.2							
		7	5th	9	326.1		22377	67.5							
		8	5th	9	326.1		21792	65.7							
		9	5th	9	326.1		22242	67.0							
15	Sealed crucible, Fe(ATrz)$_3$(NO$_3$)$_2$·H$_2$O	1	1st	9	326.4	325.8	19901	59.8							
		2	1st	9	325.1	326.1	22738	69.8	1.50	0.23	642	100.9	1.78	809	127.7
		3	1st	9	325.6	326.2	23233	70.0	1.58	-0.046	771	121.6	1.60	899	142.1
		4	3rd	9	326.2	-	23053	69.3	2.00	-0.061	868	136.9	2.07	921	145.4
		5	4th	9	326.2	-	23278	69.9	1.92	-0.188	882	139.2	2.02	998	157.6
		6	4th	9	326.2	326.2	22647	68.2	1.87	-0.19	871	137.3	1.90	966	152.6
		7	5th	9	326.0	326.1	23188	69.9	1.88	-0.54	953	150.7	1.90	966	152.6
16	Sealed crucible, Fe(ATrz)$_3$(NO$_3$)$_2$·1.25H$_2$O	1	1st	9	325.1	325.6	26095	77.5							
		2	1st	9	323.7	325.6	25504	76.8							

		3	1st	9	323.9	325.6	25458	76.7						
		4	1st	9	323.9	325.6	25458	76.7						
17	Sealed crucible, Fe(ATrz)$_3$(NO$_3$)$_2$·1.60H$_2$O	1	1st	9	321.5	322.0	25947	78.9						
		2	1st	9	318.6	321.9	26537	80.4						
		3	7th	9	318.7	322.2	27257	82.7						
18	Sealed crucible, Fe(ATrz)$_3$(NO$_3$)$_2$·6.43H$_2$O	1	1st	9	320.1	303.3	26903	83.1	1.94	2.17	646	102.6		
		2	1st	9	317.4	304.8	28382	88.2	1.83	0.94	1328	216.8	1.99	1948	319.0
		3	4th	9	318.1	303.3	28546	88.7	2.75	-4.0	2432	397.8	2.78	2432	397.9
19	Sealed crucible, Fe(ATrz)$_3$(NO$_3$)$_2$·9.96H$_2$O	1	1st	9	319.9	302.5	26845	82.4	3.32	0.27	1457	236.1	3.55	1827	296.5
		2	1st	9	317.8	301.8	27701	85.9	2.82	-0.26	1816	296.8	2.86	1970	322.2
		3	1st	9	317.7	301.4	28154	88.5	2.79	-4.0	1844	301.5	2.86	1854	303.1
20	Sealed crucible, Fe(ATrz)$_3$(NO$_3$)$_2$·14.2H$_2$O		1st	9	320.9	302.3	29427	90.5						
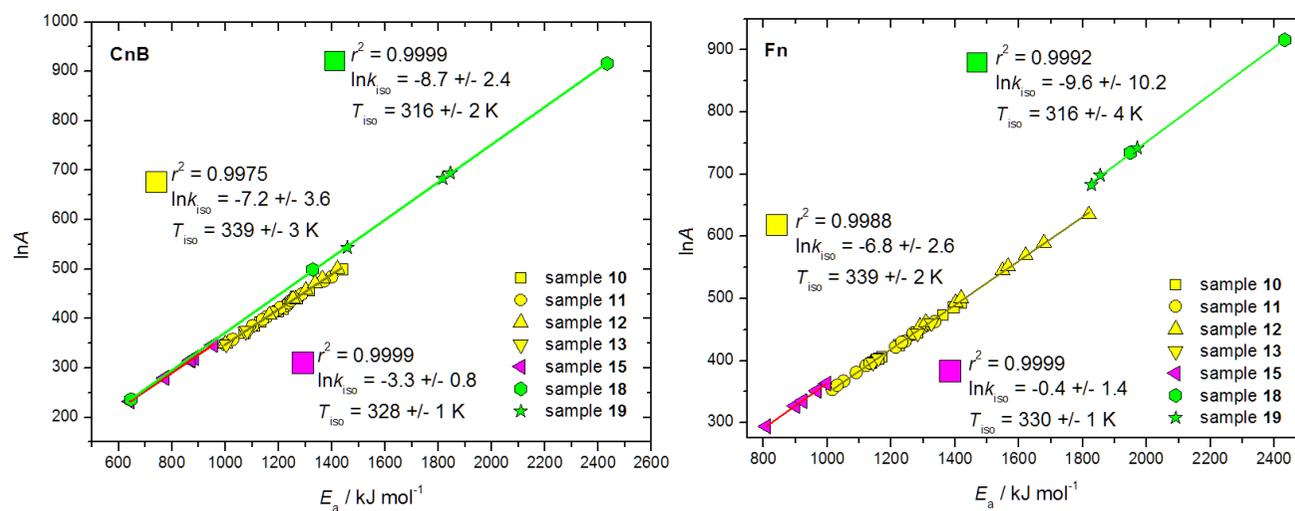
Fig S24 The $\ln A$–E_a compensation for the CnB (*left*) and Fn (*right*) models.

Table S4. The C_p values for the anhydrous complex Fe(ATrz)$_3$(NO$_3$)$_2$.

T / K	C_p / J g^{-1}	C_p / J mol^{-1}	T / K	C_p / J g^{-1}	C_p / J mol^{-1}	T / K	C_p / J g^{-1}	C_p / J mol^{-1}	T / K	C_p / J g^{-1}	C_p / J mol^{-1}
301.63	1.1435	494.11	321.83	1.4332	619.28	342.13	11.8610	5125.13	362.45	1.2575	543.36
301.92	1.1467	495.51	322.13	1.4396	622.03	342.43	10.4568	4518.36	362.75	1.2579	543.53
302.21	1.1503	497.03	322.42	1.4412	622.76	342.73	8.7674	3788.40	363.05	1.2603	544.57
302.50	1.1525	498.00	322.72	1.4437	623.81	343.03	7.0319	3038.47	363.34	1.2605	544.64
302.79	1.1536	498.47	323.02	1.4481	625.71	343.33	5.5134	2382.32	363.64	1.2598	544.34
303.09	1.1553	499.19	323.32	1.4506	626.82	343.63	4.3391	1874.93	363.94	1.2576	543.42
303.38	1.1584	500.55	323.62	1.4558	629.07	343.93	3.4971	1511.08	364.24	1.2568	543.04
303.67	1.1621	502.13	323.91	1.4625	631.95	344.22	2.9167	1260.32	364.54	1.2562	542.79
303.97	1.1686	504.96	324.21	1.4695	634.96	344.52	2.5151	1086.77	364.84	1.2538	541.78
304.26	1.1722	506.50	324.51	1.4756	637.60	344.82	2.2350	965.75	365.14	1.2524	541.17
304.56	1.1763	508.28	324.81	1.4802	639.58	345.12	2.0395	881.26	365.44	1.2539	541.80
304.86	1.1812	510.40	325.11	1.4821	640.40	345.42	1.8967	819.58	365.74	1.2552	542.38
305.15	1.1839	511.56	325.41	1.4860	642.10	345.72	1.7919	774.27	366.04	1.2577	543.45
305.45	1.1823	510.86	325.70	1.4918	644.61	346.02	1.7137	740.48	366.33	1.2592	544.09
305.75	1.1841	511.63	326.00	1.4957	646.28	346.31	1.6538	714.60	366.63	1.2586	543.84
306.05	1.1886	513.61	326.30	1.4998	648.07	346.61	1.6087	695.11	366.93	1.2583	543.69
306.34	1.1931	515.54	326.60	1.5063	650.88	346.91	1.5729	679.63	367.23	1.2606	544.69
306.64	1.1979	517.61	326.90	1.5114	653.05	347.21	1.5439	667.11	367.53	1.2632	545.81
306.94	1.2021	519.44	327.20	1.5153	654.74	347.51	1.5163	655.21	367.83	1.2634	545.92
307.23	1.2073	521.69	327.50	1.5221	657.71	347.81	1.4924	644.86	368.13	1.2643	546.29
307.53	1.2116	523.54	327.80	1.5277	660.10	348.11	1.4739	636.88	368.43	1.2654	546.79
307.83	1.2165	525.67	328.09	1.5319	661.94	348.41	1.4584	630.17	368.73	1.2648	546.51
308.13	1.2214	527.76	328.39	1.5380	664.59	348.71	1.4451	624.45	369.03	1.2661	547.08
308.42	1.2240	528.87	328.69	1.5449	667.53	349.00	1.4323	618.88	369.32	1.2678	547.82
308.72	1.2281	530.68	328.99	1.5525	670.82	349.30	1.4194	613.32	369.62	1.2688	548.26
309.02	1.2339	533.16	329.29	1.5616	674.78	349.60	1.4079	608.37	369.92	1.2674	547.63
309.32	1.2392	535.47	329.59	1.5714	678.98	349.90	1.3960	603.20	370.22	1.2630	545.73
309.62	1.2449	537.94	329.89	1.5782	681.95	350.20	1.3845	598.25	370.52	1.2577	543.47
309.92	1.2508	540.48	330.18	1.5874	685.92	350.50	1.3786	595.69	370.82	1.2582	543.65
310.21	1.2591	544.05	330.48	1.5984	690.66	350.80	1.3743	593.85	371.12	1.2614	545.05
310.51	1.2669	547.44	330.78	1.6084	694.98	351.10	1.3697	591.83	371.42	1.2624	545.49
310.81	1.2723	549.77	331.08	1.6222	700.96	351.40	1.3630	588.96	371.72	1.2624	545.48
311.11	1.2754	551.11	331.38	1.6353	706.61	351.69	1.3543	585.17	372.02	1.2629	545.68
311.41	1.2770	551.80	331.68	1.6473	711.80	351.99	1.3461	581.64	372.31	1.2595	544.22
311.70	1.2790	552.64	331.98	1.6585	716.61	352.29	1.3373	577.85	372.61	1.2549	542.25
312.00	1.2844	554.99	332.27	1.6711	722.10	352.59	1.3317	575.44	372.91	1.2543	541.97
312.30	1.2888	556.89	332.57	1.6858	728.44	352.89	1.3288	574.16	373.21	1.2532	541.51
312.60	1.2932	558.80	332.87	1.7001	734.61	353.19	1.3239	572.05	373.51	1.2512	540.64
312.89	1.2989	561.26	333.17	1.7169	741.85	353.49	1.3199	570.33	373.81	1.2523	541.10
313.19	1.3045	563.67	333.47	1.7371	750.59	353.79	1.3160	568.63	374.11	1.2529	541.36
313.49	1.3095	565.82	333.77	1.7755	759.40	354.08	1.3117	566.78	374.41	1.2513	540.66
313.79	1.3123	567.07	334.07	1.7791	768.73	354.38	1.3048	563.80	374.70	1.2490	539.67
314.08	1.3170	569.06	334.36	1.8059	780.32	354.68	1.2986	561.10	375.00	1.2495	539.93
314.38	1.3235	571.87	334.66	1.8376	794.03	354.98	1.2995	561.51	375.30	1.2528	541.33
314.68	1.3270	573.41	334.96	1.8743	809.88	355.28	1.2994	561.47	375.60	1.2542	541.95
314.98	1.3307	574.98	335.26	1.9191	829.23	355.58	1.2952	559.63	375.90	1.2506	540.39
315.28	1.3359	577.25	335.56	1.9690	850.80	355.88	1.2920	558.26	376.20	1.2500	540.12
315.57	1.3414	579.62	335.86	2.0244	874.73	356.18	1.2892	557.04	376.50	1.2529	541.38
315.87	1.3474	582.21	336.16	2.0923	904.09	356.47	1.2855	555.45	376.80	1.2523	541.10
316.17	1.3537	584.92	336.46	2.1753	939.95	356.77	1.2831	554.44	377.10	1.2523	541.14
316.47	1.3588	587.14	336.76	2.2752	983.11	357.07	1.2812	553.60	377.40	1.2554	542.46
316.76	1.3637	589.25	337.05	2.4003	1037.16	357.37	1.2796	552.90	377.69	1.2577	543.43
317.06	1.3683	591.23	337.35	2.5587	1105.62	357.67	1.2785	552.43	377.99	1.2564	542.89
317.36	1.3707	592.29	337.65	2.7651	1194.79	357.97	1.2763	551.49	378.29	1.2543	541.96
317.66	1.3755	594.33	337.95	3.0350	1311.44	358.26	1.2734	550.23	378.59	1.2531	541.45
317.95	1.3800	596.31	338.25	3.3938	1466.46	358.56	1.2708	549.10	378.89	1.2539	541.81
318.25	1.3840	598.01	338.55	3.8830	1677.83	358.86	1.2711	549.24	379.19	1.2554	542.47
318.55	1.3892	600.29	338.85	4.5639	1972.07	359.16	1.2709	549.17			
318.85	1.3934	602.10	339.14	5.5220	2386.05	359.46	1.2711	549.25			
319.15	1.3970	603.65	339.44	6.8399	2955.53	359.76	1.2701	548.81			
319.44	1.4005	605.15	339.74	8.4549	3653.37	360.06	1.2688	548.24			
319.74	1.4037	606.53	340.04	10.1124	4369.56	360.35	1.2654	546.77			
320.04	1.4092	608.91	340.34	11.5447	4988.44	360.65	1.2646	546.42			
320.34	1.4149	611.40	340.64	12.6157	5451.21	360.95	1.2662	547.11			
320.64	1.4192	613.22	340.94	13.2845	5740.23	361.25	1.2639	546.13			
320.93	1.4219	614.41	341.24	13.5492	5854.60	361.55	1.2612	544.96			
321.23	1.4216	614.29	341.53	13.4149	5796.56	361.85	1.2604	544.62			
321.53	1.4259	616.12	341.83	12.8582	5556.01	362.15	1.2594	544.16			

On determining the onset temperature of spin transition

Peaks or thermal anomalies on DSC curves can be characterized by the onset temperatures and the peak temperatures. The peak temperature is the temperature corresponding to the maximal rate of the thermal event whereas the onset temperature is the temperature at which a thermal event starts. Therefore it is preferable to use the onset temperature to compare DSC data. The onset temperature is determined by the intersection of the tangent of the peak with the baseline (Fig S25).
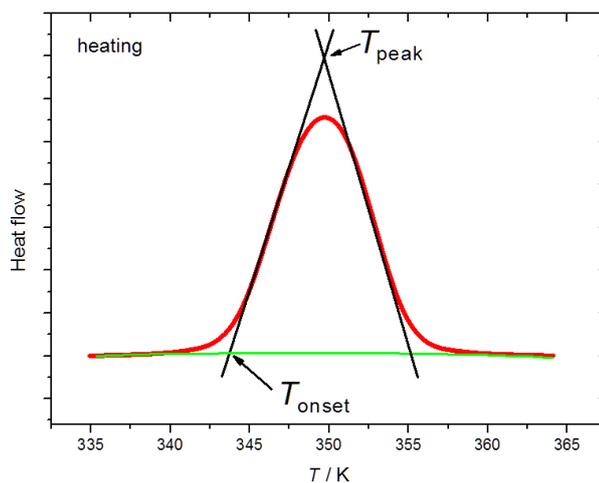
Fig. S25 How to determine the onset temperature (T_{onset}) and the peak temperature (T_{peak}) for a heating process.

On estimating entropies of spin transition

Here we would like to show our procedure of calculating entropies of spin transition. (i) The area of anomaly is divided into parts or segments (Fig. S26). (ii) Enthalpy of a segment is divided by the mean temperature of this segment. This yields entropy of this segment. (iii) Summing entropies of all segments we get entropy.

DSC /(mW/mg)
↓ exo

Partial Area: 56.49 J/g

Temperature	Partial %
322.5 K	0.000 %
323.5 K	0.036 %
324.5 K	0.179 %
325.5 K	1.081 %
326.5 K	5.347 %
327.5 K	13.717 %
328.5 K	24.186 %
329.5 K	35.325 %
330.5 K	46.532 %
331.5 K	56.795 %
332.5 K	65.423 %
333.5 K	72.918 %
334.5 K	80.195 %
335.5 K	87.115 %
336.5 K	92.489 %
337.5 K	95.777 %
338.5 K	97.588 %
339.5 K	98.590 %
340.5 K	99.179 %
341.5 K	99.534 %
342.5 K	99.752 %
343.5 K	99.880 %
344.5 K	99.948 %
345.5 K	99.982 %
346.5 K	99.996 %
347.5 K	100.000 %

Fig. S26 Dividing the thermal anomaly into segments.

Let us consider this procedure in more details. An example of calculations is shown in Fig. S27. The C1 cell (Fig. S27) is enthalpy expressed in J g^{-1}; the D1 cell is molar weight of $Fe(ATrz)_3(NO_3)_2 \cdot 1.25H_2O$. Column B (Fig. S27) is partial area of the thermal anomaly (Fig. S26) corresponding to selected temperature (Column A, Fig. S27). Column C is partial enthalpy corresponding to a segment between the ith and $(i – 1)^{th}$ temperatures. Column D is partial entropy calculated by dividing partial enthalpy corresponding to a segment between the ith and $(i – 1)^{th}$ temperatures by the mean segment temperature, $(T_i – T_{i-1})/2$. Summing all partial entropies we get entropy corresponding to the thermal anomaly (the D31 cell).

C8 f_x =C1*D1*(B8-B7)

	A	B	C	D	E	F	G	H
1	319,5		56,49	454,61				
2	320,5	0,000%	0	0				
3	321,5	0,000%	0	0				
4	322,5	0,000%	0	0				
5	323,5	0,036%	9,245131	0,028623				
6	324,5	0,179%	36,72371	0,113345				
7	325,5	1,081%	231,6419	0,712744				
8	326,5	5,347%	1095,548	3,360577				
9	327,5	13,717%	2149,493	6,573373				
10	328,5	24,186%	2688,535	8,196754				
11	329,5	35,325%	2860,598	8,694825				
12	330,5	46,532%	2878,061	8,721396				
13	331,5	56,795%	2635,633	7,962637				
14	332,5	65,423%	2215,75	6,673945				
15	333,5	72,918%	1924,785	5,780135				
16	334,5	80,195%	1868,8	5,595211				
17	335,5	87,115%	1777,12	5,304835				
18	336,5	92,489%	1380,093	4,107418				
19	337,5	95,777%	844,3886	2,505604				
20	338,5	97,588%	465,0814	1,375981				
21	339,5	98,590%	257,3228	0,759064				
22	340,5	99,179%	151,2606	0,444884				
23	341,5	99,534%	91,16726	0,267353				
24	342,5	99,752%	55,9844	0,163697				
25	343,5	99,880%	32,87158	0,095835				
26	344,5	99,948%	17,46302	0,050765				
27	345,5	99,982%	8,731512	0,025309				
28	346,5	99,996%	3,595329	0,010391				
29	347,5	100,00%	1,027237	0,00296				
30								
31			25680,92	77,52766				
32								

D8 f_x =2*C8/(A8+A7)

|	A	B	C	D	E	F	G	H
1	319,5		56,49	454,61				
2	320,5	0,000%	0	0				
3	321,5	0,000%	0	0				
4	322,5	0,000%	0	0				
5	323,5	0,036%	9,245131	0,028623				
6	324,5	0,179%	36,72371	0,113345				
7	325,5	1,081%	231,6419	0,712744				
8	326,5	5,347%	1095,548	3,360577				
9	327,5	13,717%	2149,493	6,573373				
10	328,5	24,186%	2688,535	8,196754				
11	329,5	35,325%	2860,598	8,694825				
12	330,5	46,532%	2878,061	8,721396				
13	331,5	56,795%	2635,633	7,962637				
14	332,5	65,423%	2215,75	6,673945				
15	333,5	72,918%	1924,785	5,780135				
16	334,5	80,195%	1868,8	5,595211				
17	335,5	87,115%	1777,12	5,304835				
18	336,5	92,489%	1380,093	4,107418				
19	337,5	95,777%	844,3886	2,505604				
20	338,5	97,588%	465,0814	1,375981				
21	339,5	98,590%	257,3228	0,759064				
22	340,5	99,179%	151,2606	0,444884				
23	341,5	99,534%	91,16726	0,267353				
24	342,5	99,752%	55,9844	0,163697				
25	343,5	99,880%	32,87158	0,095835				
26	344,5	99,948%	17,46302	0,050765				
27	345,5	99,982%	8,731512	0,025309				
28	346,5	99,996%	3,595329	0,010391				
29	347,5	100,00%	1,027237	0,00296				
30								
31			25680,92	77,52766				
32								

Fig. S27 Calculating entropy for the thermal anomaly depicted in Fig. S26.

On fitting the DSC curves

DSC curves as they are can be analyzed using commercially available Netzsch Thermokinetics software. These curves can be processed using either model-free or model based methods to calculate kinetic parameters. Description of this software can be found at https://www.netzsch-thermal-analysis.com/en/products-solutions/software/netzsch-advanced-software/thermokinetics/#!#c278832

General methodology of both model-free analysis and model based analysis is described in "ICTAC Kinetics Committee recommendations for performing kinetic computations on thermal analysis data" by S. Vyazovkin, A. K. Burnham, J. M. Criado, L. A. Pérez-Maqueda, C. Popescu and N. Sbirrazzuoli, *Thermochimica Acta*, 2011, **520**, 1–19.

The rate of a process, $d\alpha/dt$, depends on temperature and on the extent of conversion,

$$\frac{d\alpha}{dt} = k(T)f(\alpha),$$

where $k(T)$ is the rate constant and $f(\alpha)$ is the reaction model. In most cases the rate constant is parametrized using the well-known Arrhenius equation,

$$k(T) = Ae^{\left(-\frac{E_a}{RT}\right)}.$$

The reaction model, $f(\alpha)$, depends upon the type of reaction, *i.e.* on whether the reaction is cooperative (sigmoidal), decelerating or accelerating.

To calculate the activation energy of a process using non-isothermal DSC data it is desirable to have a series of DSC curves recorded at three or more different scan rates. We have made such experiments (sample **10**, Table S3) but, although each individual DSC curve can successfully be processed with the Netzsch Thermokinetics software, the multiple data sets cannot be fitted simultaneously (this situation is analogous to the one observed in our previous study, M. B. Bushuev, D. P. Pishchur, E. B. Nikolaenkova and V, P. Krivopalov, *Phys. Chem. Chem. Phys.*, 2016, **18**, 16690—16699.). Probably the activation barrier height and pre-exponential factor are indeed not constant for the system under discussion and vary from cycle to cycle due to evolution of the complex upon thermal cycling (not an uncommon situation for spin crossover complexes): even at one and the same scan rate we observe noticeable variations in the T_{onset} values, enthalpies and entropies of spin transition (Table S3). Therefore we consider the kinetic parameters listed in Table S3 to be estimates.

Sample 10 / cycle 3 / CnB

NETZSCH Thermokinetics   1
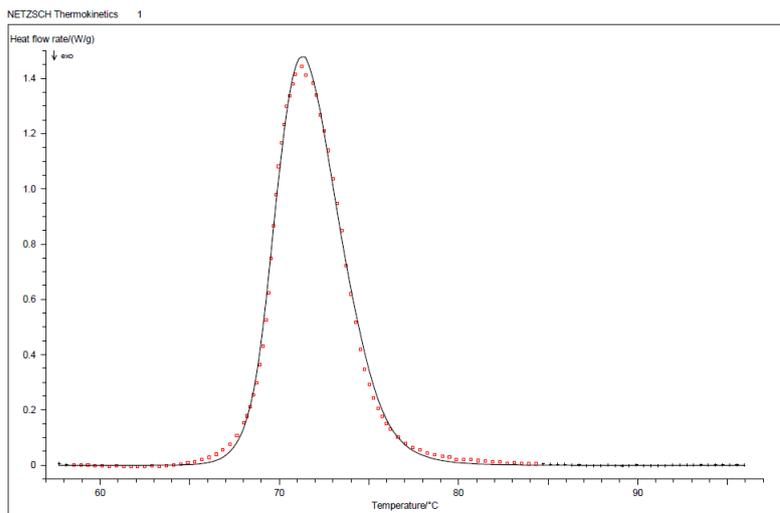
NETZSCH Thermokinetics   Date/Time: 03.10.2016 at 14:09
Project: 1
Model   1: n-th order with autocatalysis by B   A—1→B

Start evaluation:		0.00050	Measurement type:	DSC
Fine evaluation:		0.99950		
SCAN 1	Identity:		OP 320 10.11.2015 12:52:35/Segm.S1/1	
Transfer Corr:		204_F1.kcr		
Min. Temp/°C:		57.7203	Min. Time/min:	0.0
Max. Temp°C:		95.9370	Max. Time/min:	4.2651
Heating rate/(K/min):		8.960	Sampling time/s:	1.340
Sample mass/mg:		4.960		
Base line type:		tangent area prop.	LeftPts: 40	RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	62.7548	198.4512				0.5069
1	E1 kJ/mol	423.2783	1312.6495			+	3.5380
2	React.ord. 1	1.5889	2.9619			+	0.1734
3	log Kcat 1	0.4500	-2.3904				45.1319
4	Area 1/(J/g)	47.1725	47.1725				constant

STATISTICS

Least squares:	1.59459	Number of cycles:	50
Mean of residues:	9.11327E-2	Max.No of cycles:	50
Correlation coefficient:	0.998783	Rel. precision:	0.001000
Durbin-Watson Value:	0.200	t-critical(0.95;127):	1.970
Durbin-Watson Factor:	2.295		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.34	127	Bna					
1	s:	1.08	1.34	128	Fn					
2	s:	1.09	1.34	127	Cn B					
3	s:	2.27	1.34	129	B1					
4	s:	3.25	1.34	128	C1 B					
5	s:	3.63	1.34	129	F2					
6	s:	11.04	1.34	128	An					
7	s:	15.05	1.34	129	A2					
8	s:	21.49	1.34	129	F1					
9	s:	38.83	1.34	129	R3					
10	s:	46.27	1.34	129	D1F					
11	s:	49.84	1.34	129	D3F					
12	s:	51.16	1.34	129	D3					
13	s:	54.03	1.34	129	R2					
14	s:	73.45	1.34	129	D4					
15	s:	95.51	1.34	129	D2					
16	s:	141.04	1.34	129	D1					
17	s:	224.28	1.34	129	A3					

Sample 10 / cycle 4 / CnB

NETZSCH Thermokinetics 1
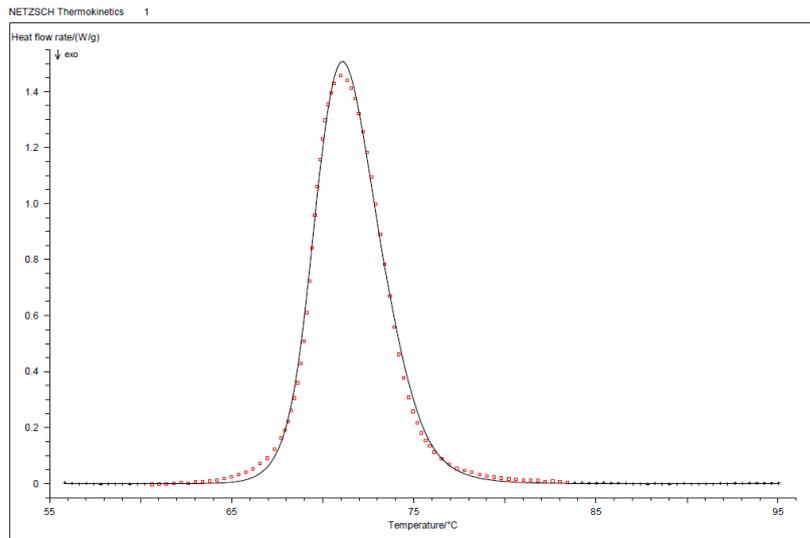
NETZSCH Thermokinetics

Date/Time: 03.10.2016 at 14:11

Project: 1
Model 1: n-th order with autocatalysis by B

A—1→B

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP 320 10.11.2015 13:42:51/Segm.S1/1
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	55.8306	Min. Time/min:	0.0
Max. Temp°C:	95.0378	Max. Time/min:	4.3764
Heating rate/(K/min):	8.959	Sampling time/s:	1.340
Sample mass/mg:	4.960		
Base line type:	tangent area prop.	LeftPts: 40	RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	66.9980	180.5794				0.8291
1	E1 kJ/mol	450.8694	1194.6979			+	5.9225
2	React.ord. 1	1.6180	2.7926			+	0.2143
3	log Kcat 1	0.4500	-0.5035				1.2490
4	Area 1/(J/g)	48.4120	48.4120				constant

STATISTICS

Least squares:	1.79563	Number of cycles:	32
Mean of residues:	9.54718E-2	Max.No of cycles:	50
Correlation coefficient:	0.998564	Rel. precision:	0.001000
Durbin-Watson Value:	0.121	t-critical(0.95;111):	1.973
Durbin-Watson Factor:	2.923		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.37	111	Bna					
1	s:	1.18	1.37	111	Cn B					
2	s:	1.19	1.37	112	Fn					
3	s:	2.38	1.37	112	C1 B					
4	s:	2.95	1.37	113	F2					
5	s:	8.23	1.37	113	B1					
6	s:	10.26	1.37	112	An					
7	s:	13.02	1.37	113	A2					
8	s:	18.93	1.37	113	F1					
9	s:	35.15	1.37	113	R3					
10	s:	41.72	1.37	113	D1F					
11	s:	45.50	1.37	113	D3F					
12	s:	46.87	1.37	113	D3					
13	s:	47.61	1.37	113	R2					
14	s:	68.23	1.37	113	D4					
15	s:	86.83	1.37	113	D2					
16	s:	131.55	1.37	113	D1					
17	s:	153.42	1.37	113	A3					

Sample 10 / cycle 5 / CnB
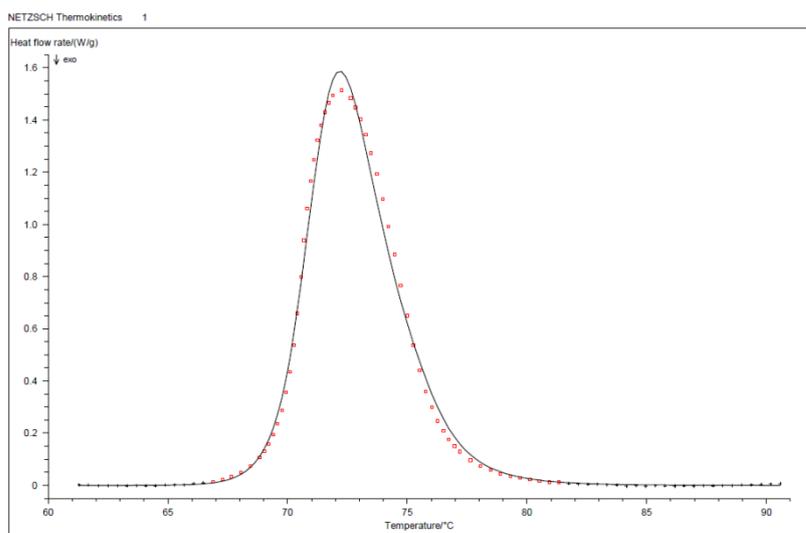
NETZSCH Thermokinetics

Date/Time: 03.10.2016 at 14:29

Project: 1
Model 1: n-th order with autocatalysis by B

A—1→B

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP 320 13.11.2015 11:11:38/Segm.S1/1		
Transfer Corr:	204_F1.kcr			
Min. Temp/°C:	61.2856	Min. Time/min:		0.0
Max. Temp°C:	90.5785	Max. Time/min:		3.2610
Heating rate/(K/min):	8.983	Sampling time/s:		1.340
Sample mass/mg:	4.880			
Base line type:	tangent area prop.	LeftPts: 25		RightPts: 40

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	36.7256	182.6888				0.4430
1	E1 kJ/mol	253.1038	1213.3336			+	4.0331
2	React.ord. 1	1.1768	3.1567			+	0.2421
3	log Kcat 1	0.4500	0.2175				0.6574
4	Area 1/(J/g)	48.7560	48.7560				constant

STATISTICS

Least squares:	4.98360	Number of cycles:	50
Mean of residues:	0.18413	Max.No of cycles:	50
Correlation coefficient:	0.996520	Rel. precision:	0.001000
Durbin-Watson Value:	0.141	t-critical(0.95;70):	1.985
Durbin-Watson Factor:	2.712		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.37	110	Bna					
1	s:	1.03	1.37	111	Fn					
2	s:	3.07	1.37	112	B1					
3	s:	3.60	1.44	70	Cn B					
4	s:	4.03	1.37	111	C1 B					
5	s:	5.12	1.37	112	F2					
6	s:	11.24	1.37	111	An					
7	s:	16.08	1.37	112	A2					
8	s:	22.79	1.37	112	F1					
9	s:	38.52	1.37	112	R3					
10	s:	46.56	1.37	112	D1F					
11	s:	49.61	1.37	112	D3F					
12	s:	50.66	1.37	112	D3					
13	s:	52.17	1.37	112	R2					
14	s:	70.27	1.37	112	D4					
15	s:	86.99	1.37	112	D2					
16	s:	113.28	1.37	112	A3					
17	s:	129.15	1.37	112	D1					

Sample 10 / cycle 6 / CnB

NETZSCH Thermokinetics   1

Heat flow rate/(W/g)

↓ exo

Temperature/°C
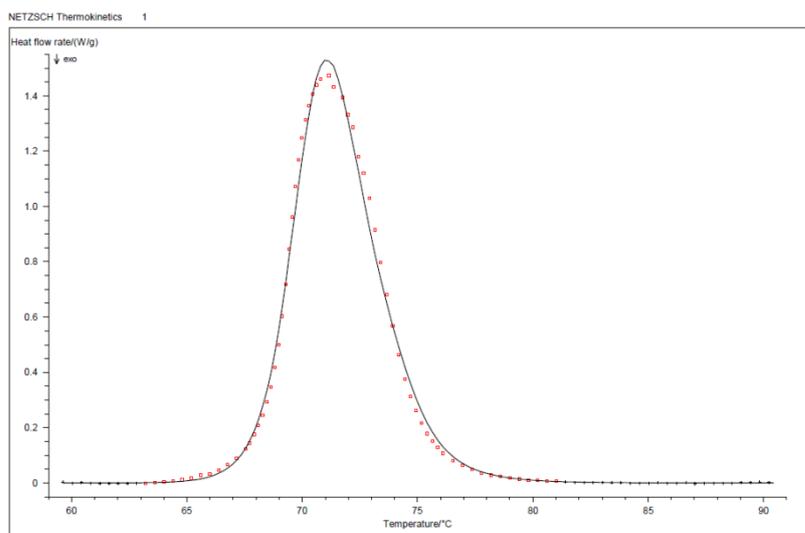
NETZSCH Thermokinetics   Date/Time: 03.10.2016 at 14:31
Project: 1
Model   1: n-th order with autocatalysis by B   A—1→B

Start evaluation:		0.00050	Measurement type:	DSC
Fine evaluation:		0.99950		
SCAN 1	Identity:		OP 320 13.11.2015 11:42:50/Segm.S1/1	
Transfer Corr:		204_F1.kcr		
Min. Temp/°C:		59.6247	Min. Time/min:	0.0
Max. Temp°C:		90.4359	Max. Time/min:	3.4390
Heating rate/(K/min):		8.959	Sampling time/s:	1.340
Sample mass/mg:		4.880		
Base line type:	tangent area prop.		LeftPts: 25	RightPts: 40

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	42.2469	161.4637				1.5885
1	E1 kJ/mol	288.5165	1069.9045			+	11.3670
2	React.ord. 1	1.2299	2.7628			+	0.2168
3	log Kcat 1	0.4500	0.1710				0.6099
4	Area 1/(J/g)	47.8679	47.8679				constant

STATISTICS

Least squares:	3.47052	Number of cycles:	50
Mean of residues:	0.14963	Max.No of cycles:	50
Correlation coefficient:	0.997607	Rel. precision:	0.001000
Durbin-Watson Value:	0.186	t-critical(0.95;86):	1.979
Durbin-Watson Factor:	2.377		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.43	86	Bna					
1	s:	1.14	1.43	87	Fn					
2	s:	1.85	1.43	86	Cn B					
3	s:	2.37	1.43	88	B1					
4	s:	2.42	1.43	87	C1 B					
5	s:	3.24	1.43	88	F2					
6	s:	8.43	1.43	87	An					
7	s:	13.85	1.43	88	A2					
8	s:	20.61	1.43	88	F1					
9	s:	37.86	1.43	88	R3					
10	s:	45.89	1.43	88	D1F					
11	s:	49.26	1.43	88	D3F					
12	s:	50.35	1.43	88	D3					
13	s:	50.92	1.43	88	R2					
14	s:	73.56	1.43	88	D4					
15	s:	91.62	1.43	88	D2					
16	s:	100.59	1.43	88	A3					
17	s:	136.16	1.43	88	D1					

Sample 10 / cycle 7 / CnB

NETZSCH Thermokinetics

Project: 1
Model 1: n-th order with autocatalysis by B

A—1→B

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP 320 16.11.2015 12:05:47/Segm.S1/1		
Transfer Corr:	204_F1.kcr			
Min. Temp/°C:	58.9123	Min. Time/min:		0.0
Max. Temp/°C:	90.1313	Max. Time/min:		3.4841
Heating rate/(K/min):	8.960	Sampling time/s:		1.340
Sample mass/mg:	4.830			
Base line type:	tangent area prop.	LeftPts: 25		RightPts: 40

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	42.7965	167.4181				0.7189
1	E1 kJ/mol	291.7231	1107.6489			+	5.7049
2	React.ord. 1	1.2320	2.8614			+	0.2088
3	log Kcat 1	0.4500	0.2228				0.5825
4	Area 1/(J/g)	49.2580	49.2580				constant

STATISTICS

Least squares:	4.61835	Number of cycles:	50
Mean of residues:	0.17151	Max.No of cycles:	50
Correlation coefficient:	0.996858	Rel. precision:	0.001000
Durbin-Watson Value:	0.138	t-critical(0.95;78):	1.982
Durbin-Watson Factor:	2.736		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.43	86	Bna					
1	s:	1.14	1.43	87	Fn					
2	s:	2.37	1.43	88	B1					
3	s:	2.42	1.43	87	C1 B					
4	s:	2.72	1.45	78	Cn B					
5	s:	3.24	1.43	88	F2					
6	s:	8.43	1.43	87	An					
7	s:	13.85	1.43	88	A2					
8	s:	20.61	1.43	88	F1					
9	s:	37.86	1.43	88	R3					
10	s:	45.89	1.43	88	D1F					
11	s:	49.26	1.43	88	D3F					
12	s:	50.35	1.43	88	D3					
13	s:	50.92	1.43	88	R2					
14	s:	73.56	1.43	88	D4					
15	s:	91.62	1.43	88	D2					
16	s:	100.59	1.43	88	A3					
17	s:	136.16	1.43	88	D1					

Sample 10 / cycle 8 / CnB

NETZSCH Thermokinetics   Date/Time: 03.10.2016 at 14:38
Project: 1
Model   1: n-th order with autocatalysis by B   A—1→B

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1	Identity:		OP 320 16.11.2015 10:59:19/Segm.S1/2	
Transfer Corr:	204_F1.kcr			
Min. Temp°C:	61.4655	Min. Time/min:		0.0
Max. Temp°C:	89.5271	Max. Time/min:		3.1371
Heating rate/(K/min):	8.945	Sampling time/s:		1.344
Sample mass/mg:	4.960			
Base line type:	tangent area prop.	LeftPts: 25		RightPts: 40

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	29.1559	217.1536				0.7047
1	E1 kJ/mol	202.8362	1437.0117			+	5.4361
2	React.ord. 1	1.0561	3.3075			+	0.3575
3	log Kcat 1	0.4500	-0.2838				1.3574
4	Area 1/(J/g)	47.5138	47.5138				constant

STATISTICS

Least squares:	4.27825	Number of cycles:		50
Mean of residues:	0.17419	Max.No of cycles:		50
Correlation coefficient:	0.997287	Rel. precision:		0.001000
Durbin-Watson Value:	0.156	t-critical(0.95;76):		1.983
Durbin-Watson Factor:	2.584			

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.43	86	Bna					
1	s:	1.14	1.43	87	Fn					
2	s:	2.37	1.43	88	B1					
3	s:	2.42	1.43	87	C1 B					
4	s:	2.59	1.45	76	Cn B					
5	s:	3.24	1.43	88	F2					
6	s:	8.43	1.43	87	An					
7	s:	13.85	1.43	88	A2					
8	s:	20.61	1.43	88	F1					
9	s:	37.86	1.43	88	R3					
10	s:	45.89	1.43	88	D1F					
11	s:	49.26	1.43	88	D3F					
12	s:	50.35	1.43	88	D3					
13	s:	50.92	1.43	88	R2					
14	s:	73.56	1.43	88	D4					
15	s:	91.62	1.43	88	D2					
16	s:	100.59	1.43	88	A3					
17	s:	136.16	1.43	88	D1					

Sample 10 / cycle 9 / CnB

NETZSCH Thermokinetics   1

NETZSCH Thermokinetics

Date/Time: 03.10.2016 at 14:34

Project: 1
Model   1: n-th order with autocatalysis by B

A—1→B

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP 320 16.11.2015 12:37:39/Segm.S1/1		
Transfer Corr:	204_F1.kcr			
Min. Temp/°C:	58.8196	Min. Time/min:		0.0
Max. Temp°C:	90.6281	Max. Time/min:		5.3235
Heating rate/(K/min):	5.975	Sampling time/s:		2.009
Sample mass/mg:	4.830			
Base line type:	tangent area prop.	LeftPts: 20		RightPts: 40

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	83.2593	198.4490				2.3612
1	E1 kJ/mol	557.5248	1311.3948			+	16.5442
2	React.ord. 1	1.6531	2.7134			+	0.2948
3	log Kcat 1	0.4500	-6.9987E-2				1.0641
4	Area 1/(J/g)	49.2407	49.2407				constant

STATISTICS

Least squares:	1.40438	Number of cycles:	24
Mean of residues:	9.36878E-2	Max.No of cycles:	50
Correlation coefficient:	0.998291	Rel. precision:	0.001000
Durbin-Watson Value:	0.179	t-critical(0.95;84):	1.980
Durbin-Watson Factor:	2.415		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.44	84	Cn B					
1	s:	1.30	1.43	86	Bna					
2	s:	1.48	1.43	87	Fn					
3	s:	3.09	1.43	88	B1					
4	s:	3.15	1.43	87	C1 B					
5	s:	4.21	1.43	88	F2					
6	s:	10.98	1.43	87	An					
7	s:	18.04	1.43	88	A2					
8	s:	26.84	1.43	88	F1					
9	s:	49.31	1.43	88	R3					
10	s:	59.76	1.43	88	D1F					
11	s:	64.16	1.43	88	D3F					
12	s:	65.58	1.43	88	D3					
13	s:	66.32	1.43	88	R2					
14	s:	95.80	1.43	88	D4					
15	s:	119.33	1.43	88	D2					
16	s:	131.01	1.43	88	A3					
17	s:	177.33	1.43	88	D1					

Sample 10 / cycle 10 / CnB
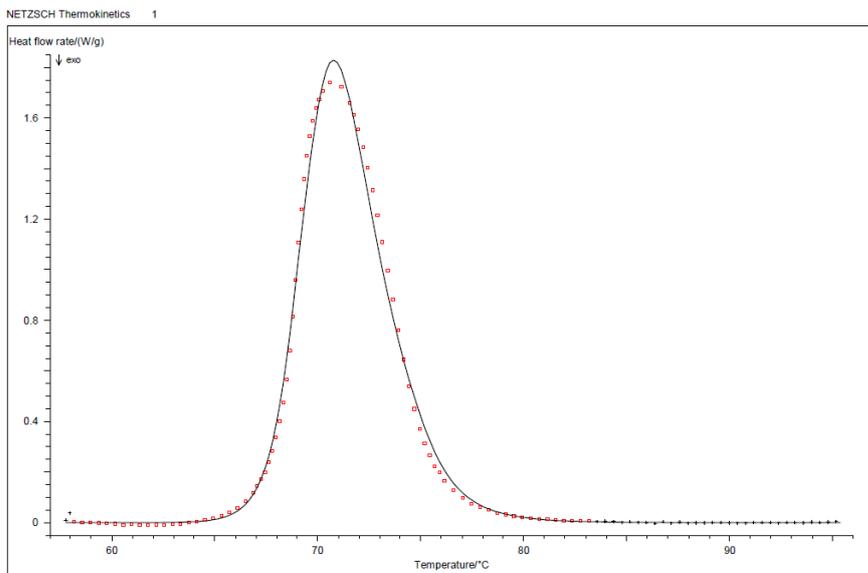
NETZSCH Thermokinetics

Project: 1
Model 1: n-th order with autocatalysis by B

Date/Time: 03.10.2016 at 14:39

A — 1 → B

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP 320 16.11.2015 13:22:15/Segm.S1/1	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	57.7655	Min. Time/min:	0.0
Max. Temp°C:	95.3703	Max. Time/min:	3.1468
Heating rate/(K/min):	11.950	Sampling time/s:	1.004
Sample mass/mg:	4.830		
Base line type:	tangent area prop.	LeftPts: 40	RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	22.1401	171.0874				0.9772
1	E1 kJ/mol	155.8758	1130.7518			+	7.3654
2	React.ord. 1	1.0209	3.1185			+	0.3182
3	log Kcat 1	0.4500	-9.7555E-2				1.0560
4	Area 1/(J/g)	48.2557	48.2557				constant

STATISTICS

Least squares:	5.60612	Number of cycles:	50
Mean of residues:	0.17223	Max.No of cycles:	50
Correlation coefficient:	0.997437	Rel. precision:	0.001000
Durbin-Watson Value:	0.117	t-critical(0.95;123):	1.970
Durbin-Watson Factor:	2.968		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.43	86	Bna					
1	s:	1.14	1.43	87	Fn					
2	s:	2.09	1.38	123	Cn B					
3	s:	2.37	1.43	88	B1					
4	s:	2.42	1.43	87	C1 B					
5	s:	3.24	1.43	88	F2					
6	s:	8.43	1.43	87	An					
7	s:	13.85	1.43	88	A2					
8	s:	20.61	1.43	88	F1					
9	s:	37.86	1.43	88	R3					
10	s:	45.89	1.43	88	D1F					
11	s:	49.26	1.43	88	D3F					
12	s:	50.35	1.43	88	D3					
13	s:	50.92	1.43	88	R2					
14	s:	73.56	1.43	88	D4					
15	s:	91.62	1.43	88	D2					
16	s:	100.59	1.43	88	A3					
17	s:	136.16	1.43	88	D1					

Sample 11 / cycle 1 / CnB

NETZSCH Thermokinetics   Date/Time: 02.10.2016 at 16:44
Project: 1
Model   1: n-th order with autocatalysis by B   A—1→B

Start evaluation:		0.00050	Measurement type:		DSC
Fine evaluation:		0.99950			
SCAN 1	Identity:		OP320 21.04.2016 17:11:05/Segm.S2/3		
Transfer Corr:		204_F1.kcr			
Min. Temp/°C:		62.4091	Min. Time/min:		0.0
Max. Temp°C:		90.6858	Max. Time/min:		3.1457
Heating rate/(K/min):		8.989	Sampling time/s:		1.339
Sample mass/mg:		3.870			
Base line type:		tangent area prop.	LeftPts: 30		RightPts: 40

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	30.4715	210.4873				2.4210E-2
1	E1 kJ/mol	212.4624	1399.5238			+	0.3253
2	React.ord. 1	0.9910	2.7788			+	0.1696
3	log Kcat 1	0.4500	-4.0000				constant
4	Area 1/(J/g)	51.5822	51.5822				constant

STATISTICS

Least squares:	4.58571	Number of cycles:		21
Mean of residues:	0.17970	Max.No of cycles:		50
Correlation coefficient:	0.997695	Rel. precision:		0.001000
Durbin-Watson Value:	0.203	t-critical(0.95;76):		1.983
Durbin-Watson Factor:	2.278			

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.46	76	Cn B					
1	s:	1.32	1.46	80	Fn					
2	s:	2.54	1.49	67	F2					
3	s:	3.06	1.49	66	C1 B					
4	s:	3.20	1.49	67	B1					
5	s:	5.83	1.49	66	An					
6	s:	8.54	1.49	67	A3					
7	s:	10.04	1.49	67	A2					
8	s:	14.54	1.49	67	F1					
9	s:	26.50	1.49	67	R3					
10	s:	32.96	1.49	67	D1F					
11	s:	34.10	1.49	67	D3F					
12	s:	34.71	1.49	67	D3					
13	s:	35.58	1.49	67	R2					
14	s:	49.95	1.49	67	D4					
15	s:	65.24	1.49	67	D2					
16	s:	95.97	1.49	67	D1					
17	s:	95.97	1.49	67	D1					

Sample 11 / cycle 2 / CnB
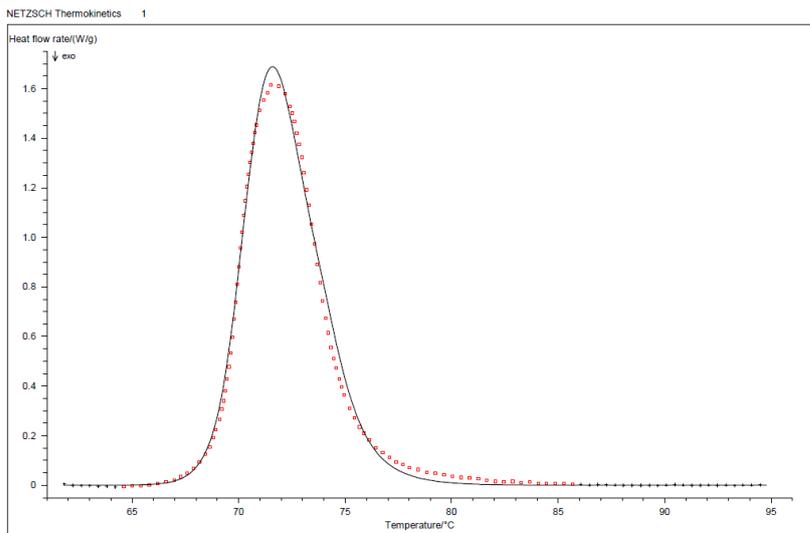
NETZSCH Thermokinetics

Date/Time: 02.10.2016 at 16:52

Project: 1
Model 1: n-th order with autocatalysis by B

A — 1→ B

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 22.04.2016 12:59:05/Segm.S1/2	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	61.8096	Min. Time/min:	0.0
Max. Temp°C:	94.7741	Max. Time/min:	3.6858
Heating rate/(K/min):	8.944	Sampling time/s:	0.672
Sample mass/mg:	3.870		
Base line type:	tangent area prop.	LeftPts: 50	RightPts: 70

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	55.7595	206.8957				0.3211
1	E1 kJ/mol	377.7323	1369.7622			+	2.3391
2	React.ord. 1	1.4398	2.9825			+	0.1688
3	log Kcat 1	0.4500	-0.8532				1.5406
4	Area 1/(J/g)	50.2248	50.2248				constant

STATISTICS

Least squares:	3.97028	Number of cycles:	23
Mean of residues:	0.10969	Max.No of cycles:	50
Correlation coefficient:	0.997668	Rel. precision:	0.001000
Durbin-Watson Value:	0.046	t-critical(0.95;208):	1.963
Durbin-Watson Factor:	4.668		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.26	208	Cn B					
1	s:	1.00	1.26	209	Fn					
2	s:	1.01	1.26	208	Bna					
3	s:	1.58	1.26	209	C1 B					
4	s:	1.72	1.26	210	B1					
5	s:	2.38	1.26	210	F2					
6	s:	5.59	1.26	209	An					
7	s:	8.61	1.26	210	A2					
8	s:	11.66	1.26	210	F1					
9	s:	20.32	1.26	210	R3					
10	s:	23.43	1.26	210	D1F					
11	s:	24.90	1.26	210	D3F					
12	s:	25.61	1.26	210	D3					
13	s:	26.93	1.26	210	R2					
14	s:	37.18	1.26	210	D4					
15	s:	46.87	1.26	210	D2					
16	s:	70.87	1.26	210	D1					
17	s:	82.55	1.26	210	A3					

Sample 11 / cycle 3 / CnB

NETZSCH Thermokinetics   1

Heat flow rate/(W/g)
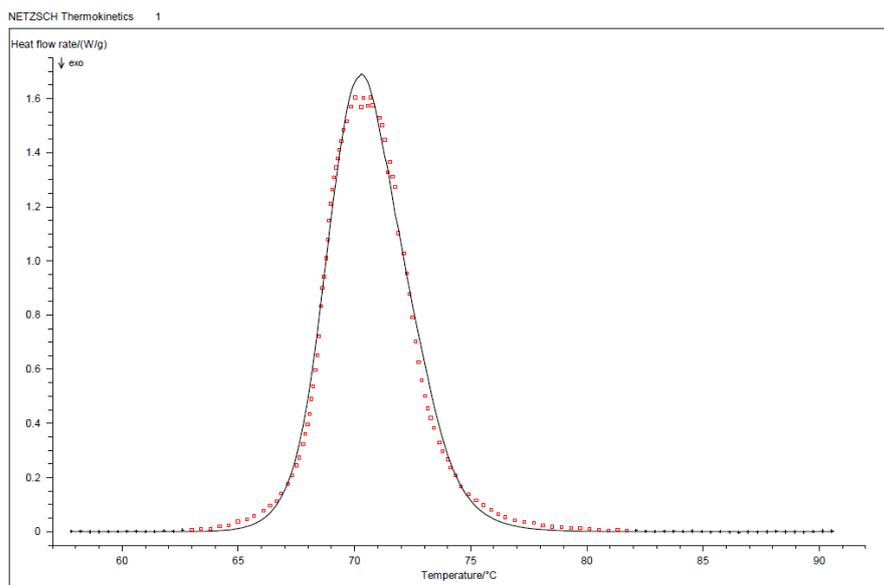
NETZSCH Thermokinetics

Date/Time: 02.10.2016 at 16:56

Project: 1
Model   1: n-th order with autocatalysis by B   A—1→B

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 22.04.2016 13:30:23/Segm.S1/2	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	57.8146	Min. Time/min:	0.0
Max. Temp°C:	90.6392	Max. Time/min:	3.6649
Heating rate/(K/min):	8.956	Sampling time/s:	0.670
Sample mass/mg:	3.870		
Base line type:	tangent area prop.	LeftPts: 40	RightPts: 70

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	35.4660	187.0035				279.0263
1	E1 kJ/mol	243.4855	1234.0123			+	3.9091E-2
2	React.ord. 1	1.0595	2.5373			+	19.8637
3	log Kcat 1	0.4500	-4.0000				constant
4	Area 1/(J/g)	50.1469	50.1469				constant

STATISTICS

Least squares:	4.38011	Number of cycles:	11
Mean of residues:	0.11538	Max.No of cycles:	50
Correlation coefficient:	0.997323	Rel. precision:	0.001000
Durbin-Watson Value:	0.195	t-critical(0.95;186):	1.964
Durbin-Watson Factor:	2.319		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.28	186	Cn B					
1	s:	1.35	1.27	188	B1					
2	s:	1.37	1.27	187	C1 B					
3	s:	1.45	1.27	188	F2					
4	s:	4.59	1.27	187	An					
5	s:	5.35	1.27	188	A3					
6	s:	6.02	1.27	188	A2					
7	s:	8.18	1.27	188	F1					
8	s:	15.27	1.27	188	R3					
9	s:	18.08	1.27	188	D1F					
10	s:	19.19	1.27	188	D3F					
11	s:	19.69	1.27	188	D3					
12	s:	20.92	1.27	188	R2					
13	s:	29.99	1.27	188	D4					
14	s:	38.82	1.27	188	D2					
15	s:	58.36	1.27	188	D1					
16	s:	58.36	1.27	188	D1					
17	s:	58.36	1.27	188	D1					

Sample 11 / cycle 4 / CnB
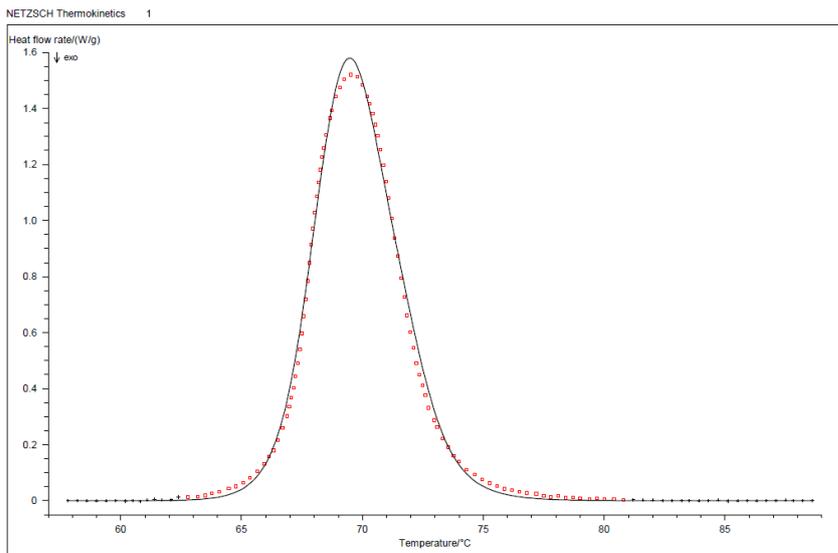
NETZSCH Thermokinetics

Date/Time: 02.10.2016 at 17:01

Project: 1
Model   1: n-th order with autocatalysis by B

A —1→ B

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP320 22.04.2016 14:15:05/Segm.S1/2		
Transfer Corr:	204_F1.kcr			
Min. Temp°C:	57.8050	Min. Time/min:		0.0
Max. Temp°C:	88.6123	Max. Time/min:		3.4425
Heating rate/(K/min):	8.949	Sampling time/s:		0.671
Sample mass/mg:	3.870			
Base line type:	tangent area prop.	LeftPts: 40		RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	46.1695	175.2195				2.3999E-2
1	E1 kJ/mol	312.8187	1154.1392			+	0.5621
2	React.ord. 1	1.2099	2.4175			+	9.4369E-2
3	log Kcat 1	0.4500	-1.3026				3.0527
4	Area 1/(J/g)	47.5889	47.5889				constant

STATISTICS

Least squares:	2.51844	Number of cycles:	23
Mean of residues:	9.02790E-2	Max.No of cycles:	50
Correlation coefficient:	0.998356	Rel. precision:	0.001000
Durbin-Watson Value:	0.052	t-critical(0.95;183):	1.964
Durbin-Watson Factor:	4.414		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.28	183	Cn B					
1	s:	2.31	1.28	188	B1					
2	s:	2.35	1.28	187	C1 B					
3	s:	2.47	1.28	188	F2					
4	s:	7.85	1.28	187	An					
5	s:	9.15	1.28	188	A3					
6	s:	10.29	1.28	188	A2					
7	s:	13.99	1.28	188	F1					
8	s:	26.12	1.28	188	R3					
9	s:	30.93	1.28	188	D1F					
10	s:	32.83	1.28	188	D3F					
11	s:	33.70	1.28	188	D3					
12	s:	35.79	1.28	188	R2					
13	s:	51.32	1.28	188	D4					
14	s:	66.42	1.28	188	D2					
15	s:	99.86	1.28	188	D1					
16	s:	99.86	1.28	188	D1					
17	s:	99.86	1.28	188	D1					

Sample 11 / cycle 5 / CnB
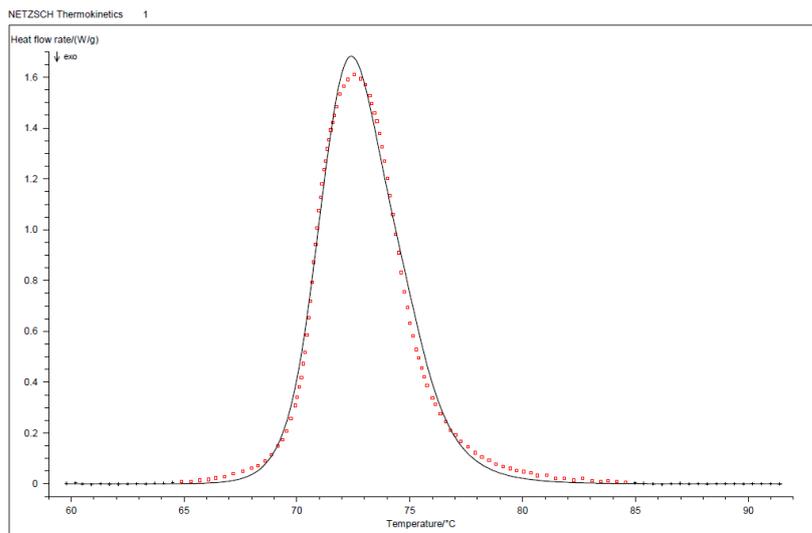
NETZSCH Thermokinetics

Project: 1
Model   1: n-th order with autocatalysis by B

A — 1 → B

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP320 26.04.2016 11:13:10/Segm.S1/2		
Transfer Corr:	204_F1.kcr			
Min. Temp/°C:	59.7870	Min. Time/min:		0.0
Max. Temp°C:	91.4874	Max. Time/min:		3.5324
Heating rate/(K/min):	8.974	Sampling time/s:		0.671
Sample mass/mg:	3.870			
Base line type:	tangent area prop.	LeftPts: 40		RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	53.0579	185.3183				2.4293E-2
1	E1 kJ/mol	360.9123	1230.8709			+	0.6147
2	React.ord. 1	1.3857	2.8544			+	0.1158
3	log Kcat 1	0.4500	-0.4033				0.5190
4	Area 1/(J/g)	51.6822	51.6822				constant

STATISTICS

Least squares:	4.71235	Number of cycles:		23
Mean of residues:	0.12192	Max.No of cycles:		50
Correlation coefficient:	0.997255	Rel. precision:		0.001000
Durbin-Watson Value:	0.047	t-critical(0.95;195):		1.963
Durbin-Watson Factor:	4.621			

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.27	195	Cn B					
1	s:	1.02	1.27	195	Bna					
2	s:	1.02	1.27	196	Fn					
3	s:	1.37	1.27	197	B1					
4	s:	1.63	1.27	196	C1 B					
5	s:	2.00	1.27	197	F2					
6	s:	5.95	1.27	196	An					
7	s:	7.46	1.27	197	A2					
8	s:	9.78	1.27	197	F1					
9	s:	17.21	1.27	197	R3					
10	s:	19.49	1.27	197	D1F					
11	s:	20.89	1.27	197	D3F					
12	s:	21.60	1.27	197	D3					
13	s:	22.92	1.27	197	R2					
14	s:	31.67	1.27	197	D4					
15	s:	39.31	1.27	197	D2					
16	s:	55.14	1.27	185	D1					
17	s:	275.20	1.27	197	A3					

Sample 11 / cycle 6 / CnB
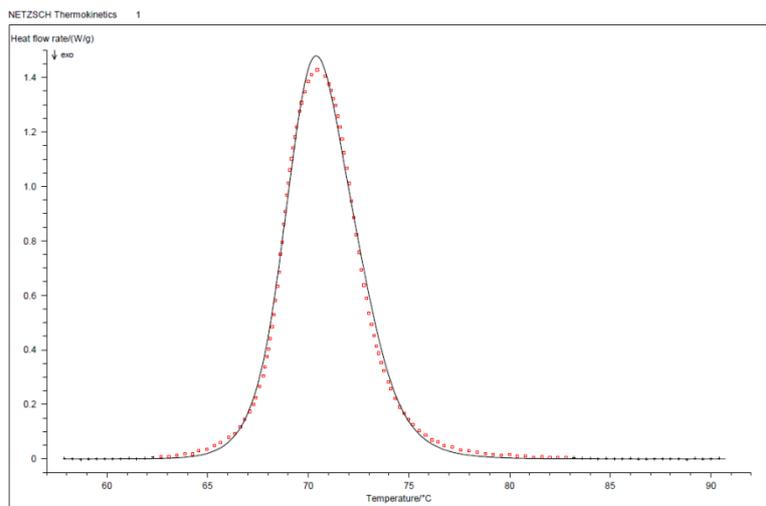
NETZSCH Thermokinetics

Date/Time: 02.10.2016 at 17:11

Project: 1
Model   1: n-th order with autocatalysis by B

A — 1 → B

Start evaluation:	0.00050		Measurement type:		DSC
Fine evaluation:	0.99950				
SCAN 1 Identity:			OP320 26.04.2016 13:08:26/Segm.S1/2		
Transfer Corr:	204_F1.kcr				
Min. Temp/°C:	57.8856		Min. Time/min:		0.0
Max. Temp°C:	90.7023		Max. Time/min:		3.6638
Heating rate/(K/min):	8.957		Sampling time/s:		0.670
Sample mass/mg:	3.870				
Base line type:	tangent area prop.		LeftPts: 40		RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	57.3191	155.3846				1.8160
1	E1 kJ/mol	386.6725	1027.5903			+	12.6136
2	React.ord. 1	1.4157	2.4459			+	0.1887
3	log Kcat 1	0.4500	-0.2153				0.9090
4	Area 1/(J/g)	45.8075	45.8075				constant

STATISTICS

Least squares:	1.95139	Number of cycles:	12
Mean of residues:	7.70148E-2	Max.No of cycles:	50
Correlation coefficient:	0.998509	Rel. precision:	0.001000
Durbin-Watson Value:	0.061	t-critical(0.95;201):	1.963
Durbin-Watson Factor:	4.087		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.26	201	Cn B					
1	s:	1.09	1.26	201	Bna					
2	s:	1.10	1.26	202	Fn					
3	s:	1.28	1.26	203	B1					
4	s:	1.43	1.26	202	C1 B					
5	s:	1.68	1.26	203	F2					
6	s:	7.39	1.26	202	An					
7	s:	9.18	1.26	203	A3					
8	s:	10.36	1.26	203	A2					
9	s:	13.66	1.26	203	F1					
10	s:	26.69	1.26	203	R3					
11	s:	29.83	1.26	203	D1F					
12	s:	31.92	1.26	203	D3F					
13	s:	33.10	1.26	203	D3					
14	s:	37.01	1.26	203	R2					
15	s:	51.77	1.26	203	D4					
16	s:	67.24	1.26	203	D2					
17	s:	105.16	1.26	203	D1					

Sample 11 / cycle 7 / CnB
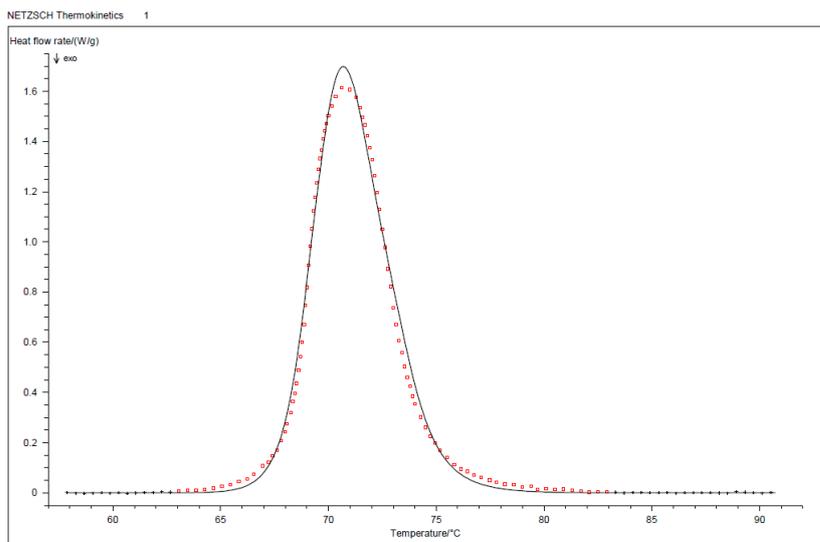
NETZSCH Thermokinetics   Date/Time: 02.10.2016 at 17:15
Project: 1
Model   1: n-th order with autocatalysis by B   A — 1 → B

Start evaluation:		0.00050	Measurement type:		DSC
Fine evaluation:		0.99950			
SCAN 1	Identity:		OP320 26.04.2016 13:49:33/Segm.S2/3		
Transfer Corr:		204_F1.kcr			
Min. Temp/°C:		57.8659	Min. Time/min:		0.0
Max. Temp°C:		90.7190	Max. Time/min:		3.6591
Heating rate/(K/min):		8.979	Sampling time/s:		0.669
Sample mass/mg:		3.770			
Base line type:		tangent area prop.	LeftPts: 40		RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	42.5377	192.8894				1.0182
1	E1 kJ/mol	290.0923	1274.2121			+	6.9993
2	React.ord. 1	1.1984	2.7396			+	0.1942
3	log Kcat 1	0.4500	-0.9027				2.1714
4	Area 1/(J/g)	50.4484	50.4484				constant

STATISTICS

Least squares:	4.34548	Number of cycles:		44
Mean of residues:	0.11493	Max.No of cycles:		50
Correlation coefficient:	0.997420	Rel. precision:		0.001000
Durbin-Watson Value:	0.055	t-critical(0.95;197):		1.963
Durbin-Watson Factor:	4.291			

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.27	197	Cn B					
1	s:	1.39	1.27	199	B1					
2	s:	1.42	1.27	198	C1 B					
3	s:	1.77	1.27	199	F2					
4	s:	5.50	1.27	198	An					
5	s:	6.99	1.27	199	A2					
6	s:	9.33	1.27	199	F1					
7	s:	16.89	1.27	199	R3					
8	s:	19.59	1.27	199	D1F					
9	s:	20.90	1.27	199	D3F					
10	s:	21.52	1.27	199	D3					
11	s:	22.77	1.27	199	R2					
12	s:	32.02	1.27	199	D4					
13	s:	40.79	1.27	199	D2					
14	s:	62.90	1.27	199	D1					
15	s:	285.74	1.27	199	A3					
16	s:	285.74	1.27	199	A3					
17	s:	285.74	1.27	199	A3					

Sample 11 / cycle 8 / CnB
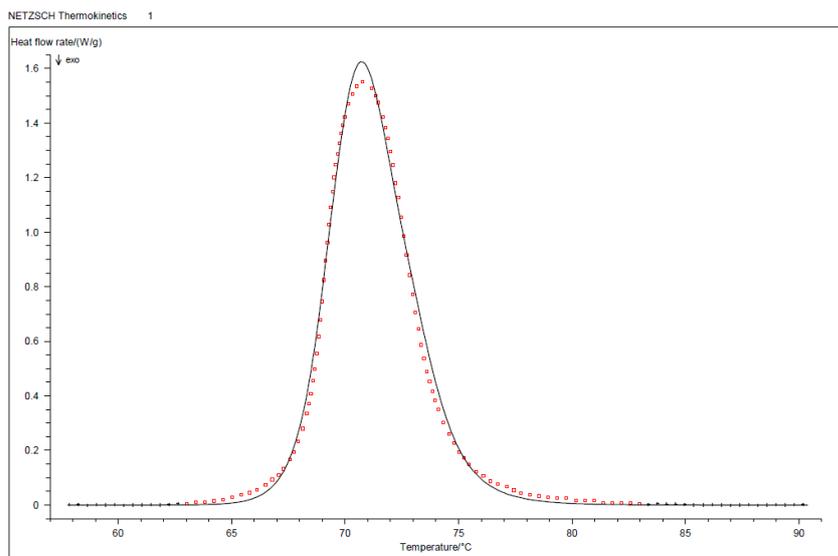
NETZSCH Thermokinetics   Date/Time: 02.10.2016 at 17:21
Project: 1
Model   1: n-th order with autocatalysis by B   A—1→B

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP320 27.04.2016 15:05:36/Segm.S1/2		
Transfer Corr:	204_F1.kcr			
Min. Temp/°C:	57.8311	Min. Time/min:		0.0
Max. Temp°C:	90.3805	Max. Time/min:		3.6398
Heating rate/(K/min):	8.943	Sampling time/s:		0.672
Sample mass/mg:	3.770			
Base line type:	tangent area prop.	LeftPts: 40		RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	48.6870	181.3198				1.1613
1	E1 kJ/mol	330.4463	1198.6221			+	8.1193
2	React.ord. 1	1.3152	2.7625			+	0.2070
3	log Kcat 1	0.4500	-0.3900				1.0141
4	Area 1/(J/g)	49.2841	49.2841				constant

STATISTICS

Least squares:	3.58504	Number of cycles:		29
Mean of residues:	0.10487	Max.No of cycles:		50
Correlation coefficient:	0.997708	Rel. precision:		0.001000
Durbin-Watson Value:	0.047	t-critical(0.95;200):		1.963
Durbin-Watson Factor:	4.624			

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.26	200	Cn B					
1	s:	1.03	1.26	201	Fn					
2	s:	1.37	1.26	202	B1					
3	s:	1.67	1.26	201	C1 B					
4	s:	1.97	1.26	202	F2					
5	s:	6.58	1.26	201	An					
6	s:	8.16	1.26	202	A2					
7	s:	10.75	1.26	202	F1					
8	s:	19.44	1.26	202	R3					
9	s:	22.06	1.26	202	D1F					
10	s:	23.67	1.26	202	D3F					
11	s:	24.43	1.26	202	D3					
12	s:	26.20	1.26	202	R2					
13	s:	36.75	1.26	202	D4					
14	s:	46.87	1.26	202	D2					
15	s:	68.84	1.26	202	D1					
16	s:	323.22	1.26	202	A3					
17	s:	323.22	1.26	202	A3					

Sample 11 / cycle 9 / CnB
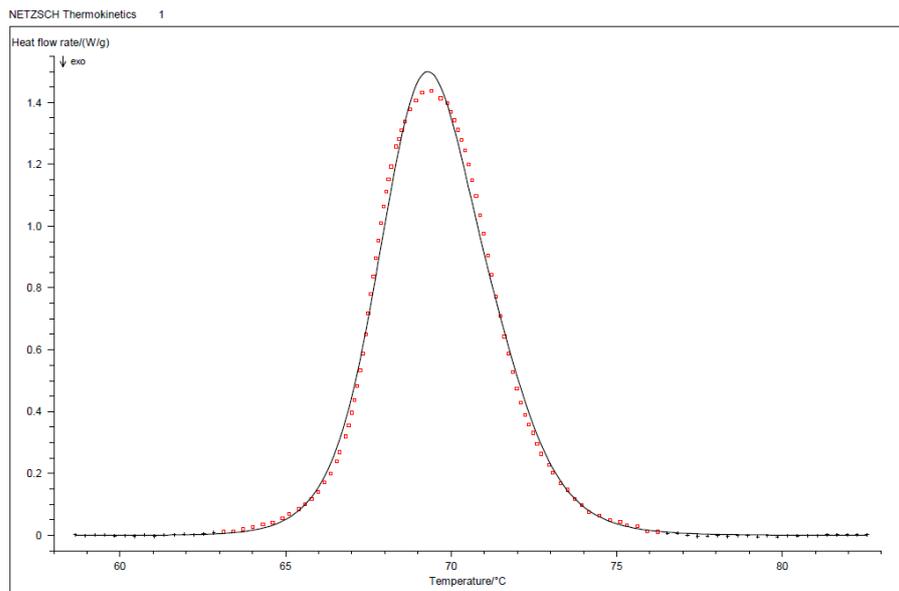
NETZSCH Thermokinetics

Date/Time: 02.10.2016 at 17:25

Project: 1
Model 1: n-th order with autocatalysis by B

$A \rightarrow 1 \rightarrow B$

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP320 27.04.2016 15:44:57/Segm.S1/2		
Transfer Corr:	204_F1.kcr			
Min. Temp/°C:	58.6448	Min. Time/min:		0.0
Max. Temp/°C:	82.5611	Max. Time/min:		2.6763
Heating rate/(K/min):	8.936	Sampling time/s:		0.672
Sample mass/mg:	3.770			
Base line type:	tangent area prop.	LeftPts: 40		RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	30.4333	167.3393				1.5886
1	E1 kJ/mol	209.9103	1102.2646			+	11.3627
2	React.ord. 1	0.9666	2.3670			+	0.2750
3	log Kcat 1	0.4500	-0.4730				2.0916
4	Area 1/(J/g)	43.9080	43.9080				constant

STATISTICS

Least squares:	3.11408	Number of cycles:	50
Mean of residues:	0.11391	Max.No of cycles:	50
Correlation coefficient:	0.997836	Rel. precision:	0.001000
Durbin-Watson Value:	0.064	t-critical(0.95;130):	1.969
Durbin-Watson Factor:	3.993		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.34	130	Cn B					
1	s:	3.80	1.30	183	An					
2	s:	5.33	1.30	184	A2					
3	s:	7.12	1.30	184	F1					
4	s:	12.03	1.30	184	A3					
5	s:	13.75	1.30	184	R3					
6	s:	15.83	1.30	184	D1F					
7	s:	16.71	1.30	184	D3F					
8	s:	17.18	1.30	184	D3					
9	s:	19.00	1.30	184	R2					
10	s:	26.30	1.30	184	D4					
11	s:	33.64	1.30	184	D2					
12	s:	52.00	1.30	184	D1					
13	s:	52.00	1.30	184	D1					
14	s:	52.00	1.30	184	D1					
15	s:	52.00	1.30	184	D1					
16	s:	52.00	1.30	184	D1					
17	s:	52.00	1.30	184	D1					

Sample 11 / cycle 10 / CnB

NETZSCH Thermokinetics   1

Heat flow rate/(W/g)
↓ exo

(x-axis: Temperature/°C, 55 65 75 85 95)
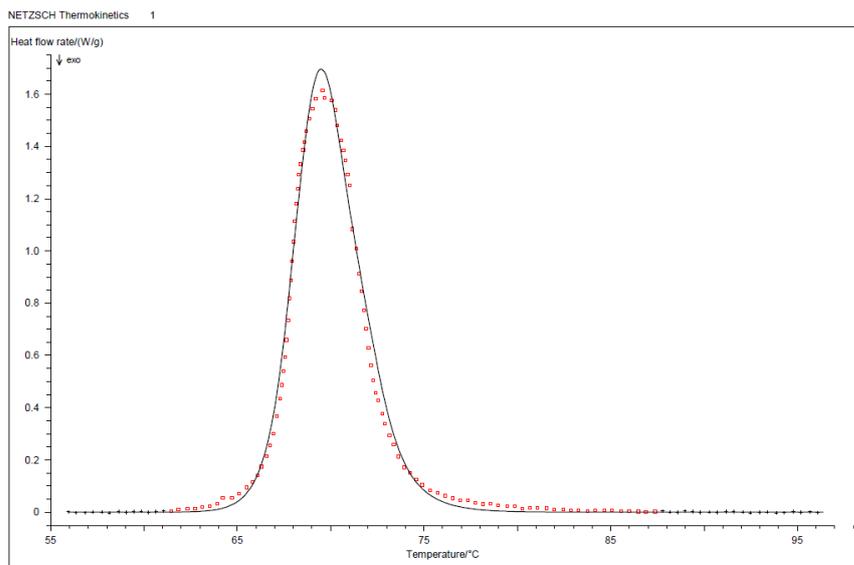
NETZSCH Thermokinetics   Date/Time: 02.10.2016 at 17:29
Project: 1
Model   1: n-th order with autocatalysis by B   A—1→B

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 27.04.2016 17:04:37/Segm.S2/3	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	55.9491	Min. Time/min:	0.0
Max. Temp°C:	96.3809	Max. Time/min:	4.5064
Heating rate/(K/min):	8.972	Sampling time/s:	0.669
Sample mass/mg:	3.770		
Base line type:	tangent area prop.	LeftPts: 40	RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	46.8888	172.9063				1.7329
1	E1 kJ/mol	317.4964	1139.4052			+	12.1518
2	React.ord. 1	1.3138	2.7248			+	0.2607
3	log Kcat 1	0.4500	-0.1786				1.0367
4	Area 1/(J/g)	51.5264	51.5264				constant

STATISTICS

Least squares:	5.21589	Number of cycles:	31
Mean of residues:	0.11348	Max.No of cycles:	50
Correlation coefficient:	0.996516	Rel. precision:	0.001000
Durbin-Watson Value:	0.105	t-critical(0.95;261):	1.960
Durbin-Watson Factor:	3.129		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.34	130	Bna					
1	s:	1.00	1.34	131	Fn					
2	s:	1.01	1.28	261	Cn B					
3	s:	1.37	1.34	132	F2					
4	s:	2.17	1.34	132	B1					
5	s:	2.19	1.34	131	C1 B					
6	s:	5.94	1.34	131	An					
7	s:	8.12	1.34	132	A3					
8	s:	9.49	1.34	132	A2					
9	s:	13.05	1.34	132	F1					
10	s:	26.36	1.34	132	R3					
11	s:	31.36	1.34	132	D1F					
12	s:	32.55	1.34	132	D3F					
13	s:	33.23	1.34	132	D3					
14	s:	36.93	1.34	132	R2					
15	s:	52.56	1.34	132	D4					
16	s:	62.67	1.30	184	D1					
17	s:	62.67	1.30	184	D1					

Sample 11 / cycle 11 / CnB
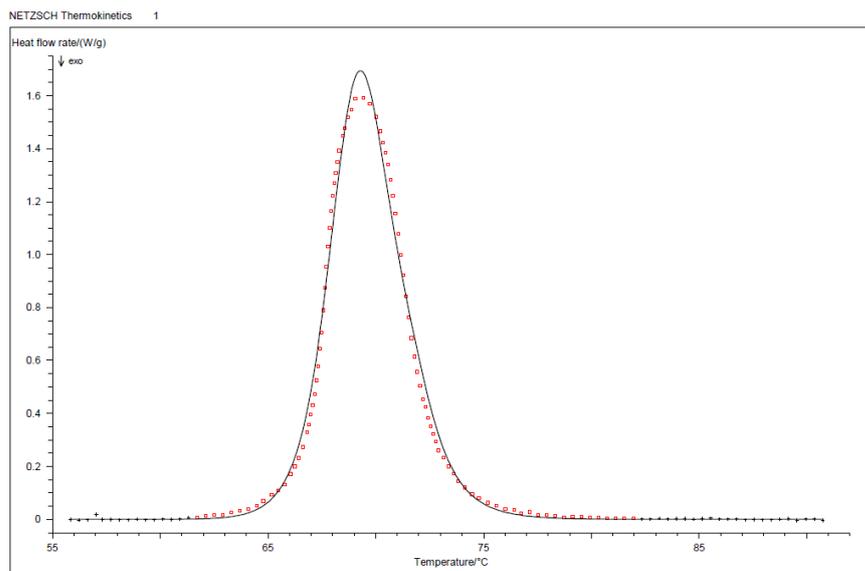
NETZSCH Thermokinetics   Date/Time: 02.10.2016 at 17:32
Project: 1
Model 1: n-th order with autocatalysis by B   A—1→B

Start evaluation:		0.00050	Measurement type:	DSC
Fine evaluation:		0.99950		
SCAN 1	Identity:		OP320 27.04.2016 17:44:40/Segm.S2/3	
Transfer Corr:		204_F1.kcr		
Min. Temp/°C:		55.8315	Min. Time/min:	0.0
Max. Temp°C:		90.7496	Max. Time/min:	3.8941
Heating rate/(K/min):		8.967	Sampling time/s:	0.669
Sample mass/mg:		3.770		
Base line type:		tangent area prop.	LeftPts: 40	RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	34.6351	151.1998				0.4708
1	E1 kJ/mol	237.3469	997.4848			+	3.6265
2	React.ord. 1	1.0605	2.4664			+	0.1049
3	log Kcat 1	0.4500	0.1725				0.3362
4	Area 1/(J/g)	50.0209	50.0209				constant

STATISTICS

Least squares:	5.22036	Number of cycles:	50
Mean of residues:	0.12213	Max.No of cycles:	50
Correlation coefficient:	0.996692	Rel. precision:	0.001000
Durbin-Watson Value:	0.058	t-critical(0.95;202):	1.963
Durbin-Watson Factor:	4.167		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.23	261	Bna					
1	s:	1.07	1.23	262	Fn					
2	s:	1.16	1.23	263	B1					
3	s:	1.34	1.25	202	Cn B					
4	s:	1.38	1.23	262	C1 B					
5	s:	1.59	1.23	263	F2					
6	s:	4.27	1.23	262	An					
7	s:	4.62	1.23	263	A3					
8	s:	5.10	1.23	263	A2					
9	s:	6.68	1.23	263	F1					
10	s:	11.78	1.23	263	R3					
11	s:	13.42	1.23	263	D1F					
12	s:	14.44	1.23	263	D3F					
13	s:	14.91	1.23	263	D3					
14	s:	15.79	1.23	263	R2					
15	s:	22.22	1.23	263	D4					
16	s:	28.19	1.23	263	D2					
17	s:	42.00	1.23	263	D1					

Sample 11 / cycle 12 / CnB
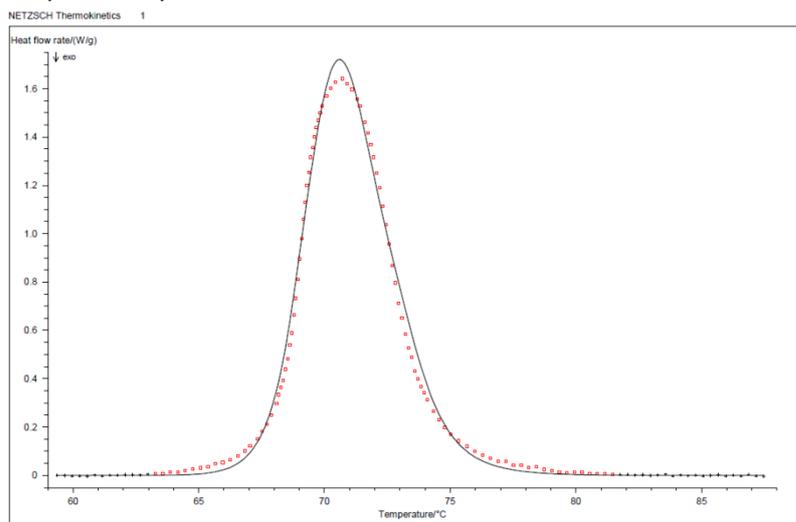
NETZSCH Thermokinetics

Date/Time: 02.10.2016 at 17:38

Project: 1
Model   1: n-th order with autocatalysis by B

A — 1 → B

Start evaluation:		0.00050	Measurement type:	DSC
Fine evaluation:		0.99950		
SCAN 1	Identity:		OP320 28.04.2016 12:45:11/Segm.S2/3	
Transfer Corr:		204_F1.kcr		
Min. Temp/°C:		59.3591	Min. Time/min:	0.0
Max. Temp°C:		87.4660	Max. Time/min:	3.1264
Heating rate/(K/min):		8.990	Sampling time/s:	0.670
Sample mass/mg:		3.770		
Base line type:		tangent area prop.	LeftPts: 30	RightPts: 40

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	39.8349	192.9430				1.3465
1	E1 kJ/mol	272.2654	1274.2760			+	9.2567
2	React.ord. 1	1.1552	2.7576			+	0.2210
3	log Kcat 1	0.4500	-0.6066				1.4470
4	Area 1/(J/g)	50.4243	50.4243				constant

STATISTICS

Least squares:	5.54808	Number of cycles:	30
Mean of residues:	0.14051	Max.No of cycles:	50
Correlation coefficient:	0.997094	Rel. precision:	0.001000
Durbin-Watson Value:	0.055	t-critical(0.95;179):	1.964
Durbin-Watson Factor:	4.313		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.26	202	Bna					
1	s:	1.06	1.26	203	Fn					
2	s:	1.31	1.26	204	B1					
3	s:	1.33	1.26	203	C1 B					
4	s:	1.46	1.26	204	F2					
5	s:	1.48	1.27	179	Cn B					
6	s:	4.68	1.26	203	An					
7	s:	5.78	1.26	204	A2					
8	s:	7.80	1.26	204	F1					
9	s:	14.61	1.26	204	R3					
10	s:	17.19	1.26	204	D1F					
11	s:	18.26	1.26	204	D3F					
12	s:	18.78	1.26	204	D3					
13	s:	20.05	1.26	204	R2					
14	s:	28.51	1.26	204	D4					
15	s:	31.31	1.26	204	A3					
16	s:	37.27	1.26	204	D2					
17	s:	57.65	1.26	204	D1					

Sample 11 / cycle 13 / CnB

NETZSCH Thermokinetics   1
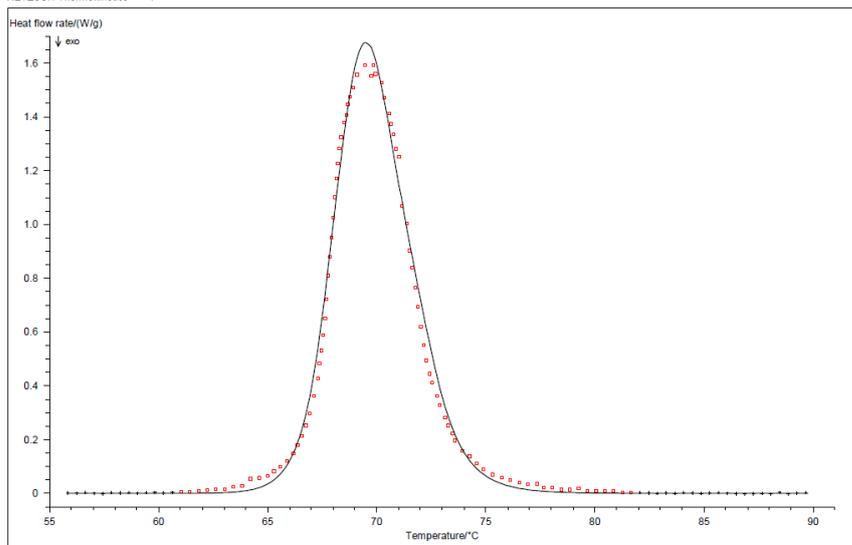
Heat flow rate/(W/g)

NETZSCH Thermokinetics

Project: 1
Model   1: n-th order with autocatalysis by B

Date/Time: 02.10.2016 at 17:44

$A \longrightarrow 1 \rightarrow B$

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP320 27.04.2016 17:04:37/Segm.S2/3		
Transfer Corr:	204_F1.kcr			
Min. Temp/°C:	55.8393	Min. Time/min:		0.0
Max. Temp°C:	89.7693	Max. Time/min:		3.7815
Heating rate/(K/min):	8.973	Sampling time/s:		0.669
Sample mass/mg:	3.770			
Base line type:	tangent area prop.	LeftPts: 40		RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	30.6365	183.1905				0.8524
1	E1 kJ/mol	211.3916	1206.3381			+	6.0023
2	React.ord. 1	1.0131	2.5993			+	0.2163
3	log Kcat 1	0.4500	-0.9058				2.7266
4	Area 1/(J/g)	50.1685	50.1685				constant

STATISTICS

Least squares:	5.09135	Number of cycles:	35
Mean of residues:	0.12237	Max.No of cycles:	50
Correlation coefficient:	0.996852	Rel. precision:	0.001000
Durbin-Watson Value:	0.139	t-critical(0.95;205):	1.963
Durbin-Watson Factor:	2.732		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.26	205	Cn B					
1	s:	1.18	1.27	179	Bna					
2	s:	1.25	1.27	180	Fn					
3	s:	1.49	1.27	181	B1					
4	s:	1.58	1.27	180	C1 B					
5	s:	2.16	1.27	181	F2					
6	s:	5.59	1.27	180	An					
7	s:	7.89	1.27	181	A2					
8	s:	10.76	1.27	181	F1					
9	s:	19.37	1.27	181	R3					
10	s:	22.52	1.27	181	D1F					
11	s:	24.15	1.27	181	D3F					
12	s:	24.87	1.27	181	D3					
13	s:	26.12	1.27	181	R2					
14	s:	36.94	1.27	181	D4					
15	s:	46.99	1.27	181	D2					
16	s:	58.06	1.27	181	A3					
17	s:	69.70	1.27	181	D1					

Sample 11 / cycle 14 / CnB
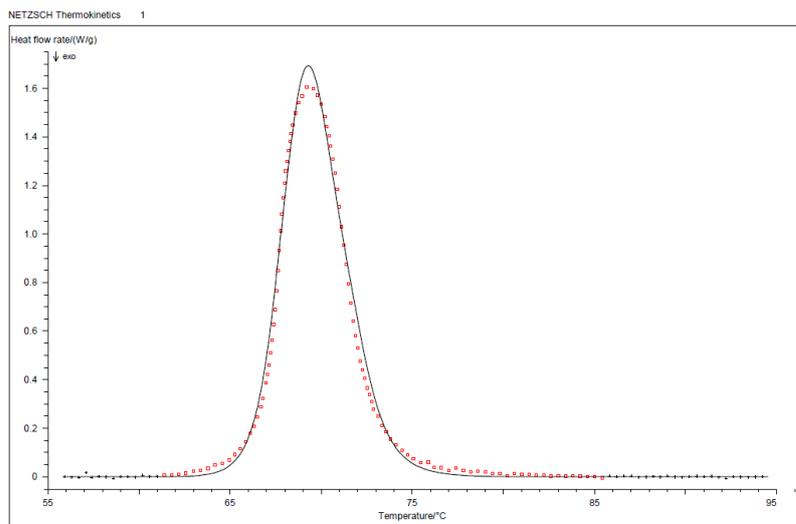
NETZSCH Thermokinetics

Project: 1
Model 1: n-th order with autocatalysis by B

Date/Time: 02.10.2016 at 17:48

A —1→ B

Start evaluation:	0.00050	Measurement type: DSC
Fine evaluation:	0.99950	
SCAN 1 Identity:		OP320 27.04.2016 17:44:40/Segm.S2/3
Transfer Corr:	204_F1.kcr	
Min. Temp/°C:	55.9012	Min. Time/min: 0.0
Max. Temp°C:	94.5206	Max. Time/min: 4.3069
Heating rate/(K/min):	8.967	Sampling time/s: 0.669
Sample mass/mg:	3.770	
Base line type:	tangent area prop.	LeftPts: 40 RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	39.1792	178.8506				1.4534
1	E1 kJ/mol	266.9950	1177.3514			+	9.9749
2	React.ord. 1	1.1534	2.5906			+	0.2131
3	log Kcat 1	0.4500	-0.5882				1.4840
4	Area 1/(J/g)	50.6936	50.6936				constant

STATISTICS

Least squares:	4.50257	Number of cycles:	34
Mean of residues:	0.10786	Max.No of cycles:	50
Correlation coefficient:	0.997052	Rel. precision:	0.001000
Durbin-Watson Value:	0.054	t-critical(0.95;237):	1.961
Durbin-Watson Factor:	4.347		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.24	237	Cn B					
1	s:	1.24	1.25	205	Bna					
2	s:	1.30	1.25	206	Fn					
3	s:	1.57	1.25	207	B1					
4	s:	1.75	1.25	206	C1 B					
5	s:	1.86	1.25	207	F2					
6	s:	5.72	1.25	206	An					
7	s:	6.88	1.25	207	A2					
8	s:	9.17	1.25	207	F1					
9	s:	16.78	1.25	207	R3					
10	s:	19.63	1.25	207	D1F					
11	s:	20.87	1.25	207	D3F					
12	s:	21.47	1.25	207	D3					
13	s:	22.88	1.25	207	R2					
14	s:	32.38	1.25	207	D4					
15	s:	41.41	1.25	207	D2					
16	s:	62.66	1.25	207	D1					
17	s:	302.01	1.25	207	A3					

Sample 11 / cycle 15 / CnB

NETZSCH Thermokinetics   1

Heat flow rate/(W/g)

↓ exo

(plot with temperature axis 60, 70, 80, 90 Temperature/°C; y-axis 0, 0.4, 0.8, 1.2, 1.6)
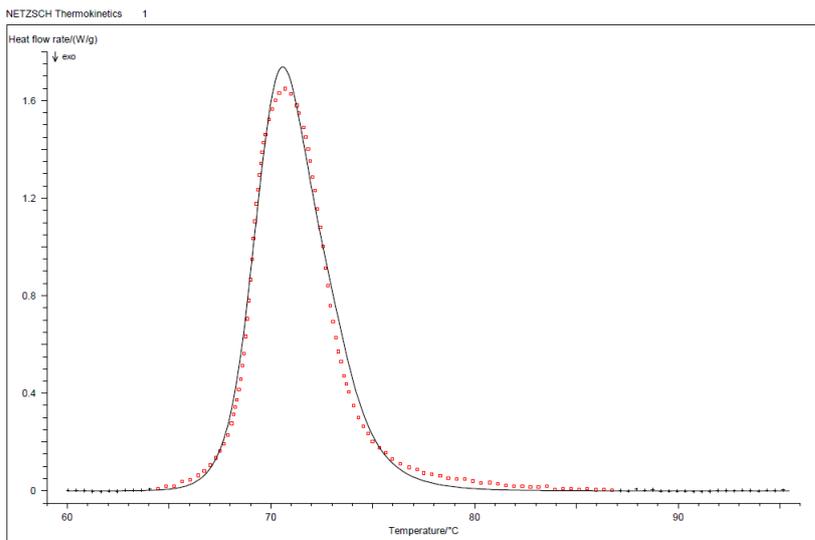
NETZSCH Thermokinetics

Date/Time: 02.10.2016 at 17:53

Project: 1
Model   1: n-th order with autocatalysis by B   A —1→ B

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		

SCAN 1   Identity: OP320 28.04.2016 12:45:11/Segm.S2/3

Transfer Corr:	204 F1.kcr		
Min. Temp/°C:	60.0415	Min. Time/min:	0.0
Max. Temp/°C:	95.4517	Max. Time/min:	3.9418
Heating rate/(K/min):	8.983	Sampling time/s:	0.670
Sample mass/mg:	3.770		
Base line type:	tangent area prop.	LeftPts: 40	RightPts: 70

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	59.4713	187.3538				0.7175
1	E1 kJ/mol	400.8909	1237.9731			+	5.3929
2	React.ord. 1	1.5630	3.0769			+	0.2411
3	log Kcat 1	0.4500	-1.3129E-2				0.6783
4	Area 1/(J/g)	52.0740	52.0740				constant

STATISTICS

Least squares:	5.98057	Number of cycles:	4
Mean of residues:	0.12998	Max.No of cycles:	50
Correlation coefficient:	0.996389	Rel. precision:	0.001000
Durbin-Watson Value:	0.044	t-critical(0.95;219):	1.962
Durbin-Watson Factor:	4.767		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.25	219	Cn B					
1	s:	1.05	1.25	219	Bna					
2	s:	1.07	1.25	220	Fn					
3	s:	1.16	1.25	221	B1					
4	s:	2.11	1.25	221	F2					
5	s:	2.73	1.25	220	C1 B					
6	s:	4.27	1.25	220	An					
7	s:	6.08	1.25	221	A2					
8	s:	8.00	1.25	221	F1					
9	s:	13.36	1.25	221	R3					
10	s:	14.84	1.25	221	D1F					
11	s:	16.19	1.25	221	D3F					
12	s:	16.76	1.25	221	D3					
13	s:	17.45	1.25	221	R2					
14	s:	24.04	1.25	221	D4					
15	s:	29.58	1.25	221	D2					
16	s:	38.73	1.25	221	A3					
17	s:	42.98	1.25	221	D1					

Sample 11 / cycle 16 / CnB
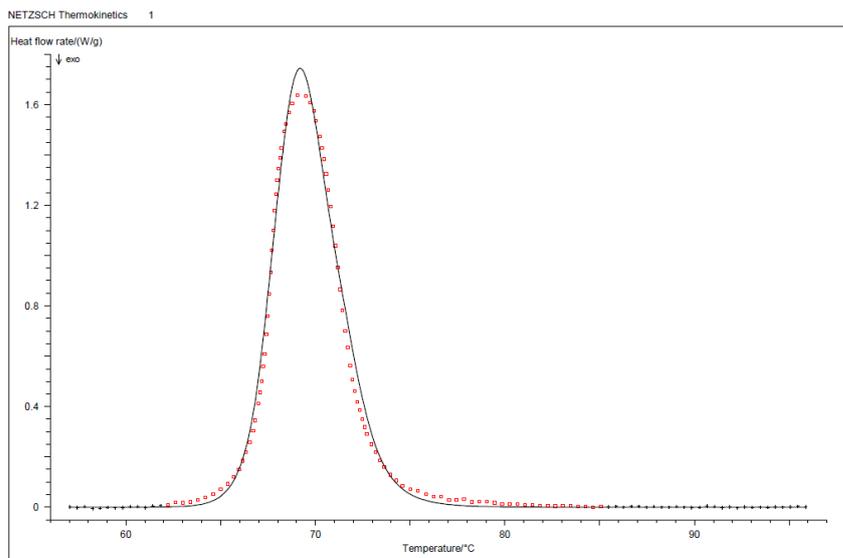
NETZSCH Thermokinetics

Date/Time: 02.10.2016 at 17:57

Project: 1
Model   1: n-th order with autocatalysis by B

A — 1 → B

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 28.04.2016 13:26:28/Segm.S2/3
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	57.0347	Min. Time/min:	0.0
Max. Temp/°C:	95.8662	Max. Time/min:	4.3287
Heating rate/(K/min):	8.971	Sampling time/s:	0.669
Sample mass/mg:	3.770		
Base line type:	tangent area prop.	LeftPts: 40	RightPts: 70

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	36.3941	189.4939				0.7881
1	E1 kJ/mol	248.6875	1246.5521			+	5.6927
2	React.ord. 1	1.1184	2.7016			+	0.2286
3	log Kcat 1	0.4500	-0.5424				1.5076
4	Area 1/(J/g)	51.0304	51.0304				constant

STATISTICS

Least squares:	5.06572	Number of cycles:	50
Mean of residues:	0.11412	Max.No of cycles:	50
Correlation coefficient:	0.996776	Rel. precision:	0.001000
Durbin-Watson Value:	0.055	t-critical(0.95;228):	1.961
Durbin-Watson Factor:	4.306		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.25	228	Bna					
1	s:	1.06	1.24	229	Fn					
2	s:	1.07	1.25	228	Cn B					
3	s:	1.28	1.24	230	B1					
4	s:	1.30	1.24	229	C1 B					
5	s:	1.59	1.24	230	F2					
6	s:	4.24	1.24	229	An					
7	s:	5.36	1.24	230	A2					
8	s:	7.29	1.24	230	F1					
9	s:	13.13	1.24	230	R3					
10	s:	15.48	1.24	230	D1F					
11	s:	16.53	1.24	230	D3F					
12	s:	16.99	1.24	230	D3					
13	s:	17.78	1.24	230	R2					
14	s:	25.20	1.24	230	D4					
15	s:	31.45	1.24	230	D2					
16	s:	47.95	1.24	230	D1					
17	s:	229.14	1.24	230	A3					

Sample 11 / cycle 17 / CnB
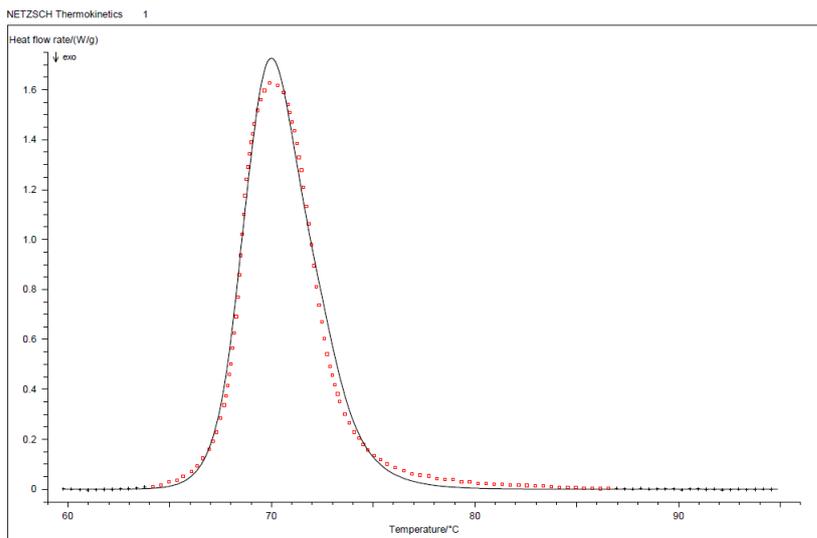
NETZSCH Thermokinetics

Date/Time: 02.10.2016 at 17:59

Project: 1
Model 1: n-th order with autocatalysis by B

$A \longrightarrow 1 \rightarrow B$

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 28.04.2016 16:37:10/Segm.S1/2	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	59.7814	Min. Time/min:	0.0
Max. Temp°C:	94.8563	Max. Time/min:	3.9119
Heating rate/(K/min):	8.966	Sampling time/s:	0.671
Sample mass/mg:	3.770		
Base line type:	tangent area prop.	LeftPts: 40	RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	53.9354	195.0287				1.2010
1	E1 kJ/mol	363.9683	1285.8932			+	8.4660
2	React.ord. 1	1.4522	3.0102			+	0.2460
3	log Kcat 1	0.4500	-0.2241				0.8915
4	Area 1/(J/g)	50.9006	50.9006				constant

STATISTICS

Least squares:	5.68664	Number of cycles:	29
Mean of residues:	0.12728	Max.No of cycles:	50
Correlation coefficient:	0.996587	Rel. precision:	0.001000
Durbin-Watson Value:	0.045	t-critical(0.95;223):	1.962
Durbin-Watson Factor:	4.747		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.25	228	Bna					
1	s:	1.06	1.24	229	Fn					
2	s:	1.23	1.25	223	Cn B					
3	s:	1.28	1.24	230	B1					
4	s:	1.30	1.24	229	C1 B					
5	s:	1.59	1.24	230	F2					
6	s:	4.24	1.24	229	An					
7	s:	5.36	1.24	230	A2					
8	s:	7.29	1.24	230	F1					
9	s:	13.13	1.24	230	R3					
10	s:	15.48	1.24	230	D1F					
11	s:	16.53	1.24	230	D3F					
12	s:	16.99	1.24	230	D3					
13	s:	17.78	1.24	230	R2					
14	s:	25.20	1.24	230	D4					
15	s:	31.45	1.24	230	D2					
16	s:	47.95	1.24	230	D1					
17	s:	229.14	1.24	230	A3					

NETZSCH Thermokinetics   1

NETZSCH Thermokinetics

Date/Time: 02.10.2016 at 18:17

Project: 1
Model   1: n-th order with autocatalysis by B   A—1→B

Start evaluation:		0.00050	Measurement type:		DSC
Fine evaluation:		0.99950			
SCAN 1	Identity:		OP320 08.05.2016 16:43:02/Segm.S2/3		
Transfer Corr:		204_F1.kcr			
Min. Temp/°C:		58.3092	Min. Time/min:		0.0
Max. Temp°C:		94.4401	Max. Time/min:		6.0408
Heating rate/(K/min):		5.981	Sampling time/s:		1.004
Sample mass/mg:		3.580			
Base line type:		tangent area prop.	LeftPts: 40		RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	111.2664	190.7843				0.2817
1	E1 kJ/mol	741.3758	1263.1556			+	2.1976
2	React.ord. 1	1.8374	2.5795			+	7.3778E-2
3	log Kcat 1	0.4500	0.5034				0.1442
4	Area 1/(J/g)	53.1013	53.1013				constant

STATISTICS

Least squares:	2.88370	Number of cycles:		30
Mean of residues:	8.92526E-2	Max.No of cycles:		50
Correlation coefficient:	0.997413	Rel. precision:		0.001000
Durbin-Watson Value:	0.075	t-critical(0.95;221):		1.962
Durbin-Watson Factor:	3.693			

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.25	221	Cn B					
1	s:	1.59	1.25	228	Bna					
2	s:	1.69	1.25	229	Fn					
3	s:	2.04	1.25	230	B1					
4	s:	2.07	1.25	229	C1 B					
5	s:	2.53	1.25	230	F2					
6	s:	6.75	1.25	229	An					
7	s:	8.53	1.25	230	A2					
8	s:	11.60	1.25	230	F1					
9	s:	20.89	1.25	230	R3					
10	s:	24.63	1.25	230	D1F					
11	s:	26.32	1.25	230	D3F					
12	s:	27.04	1.25	230	D3					
13	s:	28.30	1.25	230	R2					
14	s:	40.12	1.25	230	D4					
15	s:	50.07	1.25	230	D2					
16	s:	76.34	1.25	230	D1					
17	s:	364.77	1.25	230	A3					

Sample 12 / cycle 2 / CnB

NETZSCH Thermokinetics   1
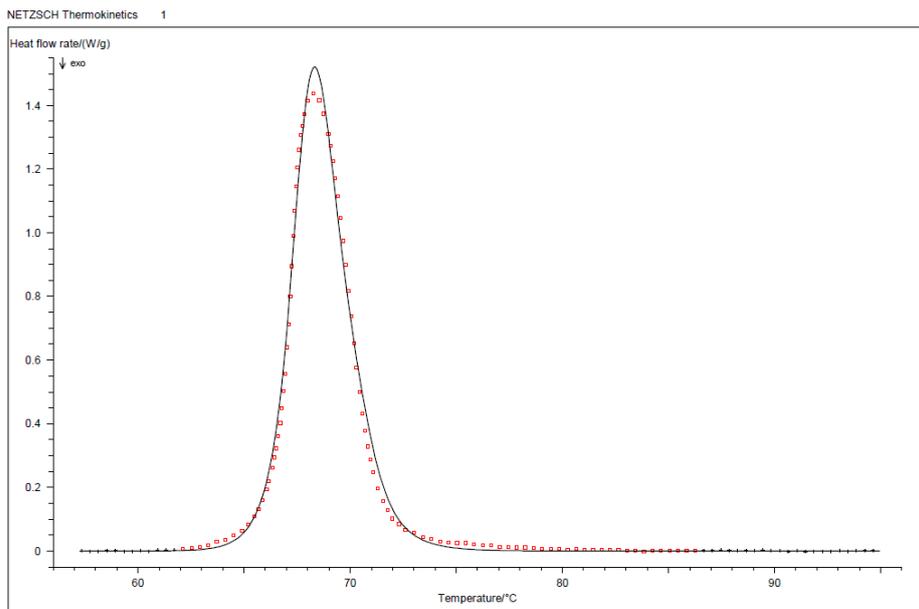
NETZSCH Thermokinetics   Date/Time: 02.10.2016 at 18:18
Project: 1
Model   1: n-th order with autocatalysis by B   A—1→B

Start evaluation:	0.00050	Measurement type:			DSC
Fine evaluation:	0.99950				
SCAN 1 Identity:		OP320 08.05.2016 17:31:51/Segm.S2/3			
Transfer Corr:	204_F1.kcr				
Min. Temp/°C:	57.3295	Min. Time/min:			0.0
Max. Temp°C:	94.9516	Max. Time/min:			6.2932
Heating rate/(K/min):	5.978	Sampling time/s:			1.004
Sample mass/mg:	3.510				
Base line type:	tangent area prop.	LeftPts: 40		RightPts: 50	

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	103.4500	177.0302				0.2624
1	E1 kJ/mol	685.4585	1165.1359			+	2.0285
2	React.ord. 1	1.8157	2.5081			+	6.8714E-2
3	log Kcat 1	0.4500	0.5328				0.1287
4	Area 1/(J/g)	51.9763	51.9763				constant

STATISTICS

Least squares:	2.66993	Number of cycles:	46
Mean of residues:	8.41549E-2	Max.No of cycles:	50
Correlation coefficient:	0.997387	Rel. precision:	0.001000
Durbin-Watson Value:	0.073	t-critical(0.95;239):	1.961
Durbin-Watson Factor:	3.727		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.24	239	Cn B					
1	s:	1.86	1.24	228	Bna					
2	s:	1.97	1.24	229	Fn					
3	s:	2.38	1.24	230	B1					
4	s:	2.42	1.24	229	C1 B					
5	s:	2.96	1.24	230	F2					
6	s:	7.89	1.24	229	An					
7	s:	9.97	1.24	230	A2					
8	s:	13.55	1.24	230	F1					
9	s:	24.41	1.24	230	R3					
10	s:	28.77	1.24	230	D1F					
11	s:	30.74	1.24	230	D3F					
12	s:	31.59	1.24	230	D3					
13	s:	33.05	1.24	230	R2					
14	s:	46.86	1.24	230	D4					
15	s:	58.48	1.24	230	D2					
16	s:	89.16	1.24	230	D1					
17	s:	426.06	1.24	230	A3					

Sample 12 / cycle 3 / CnB
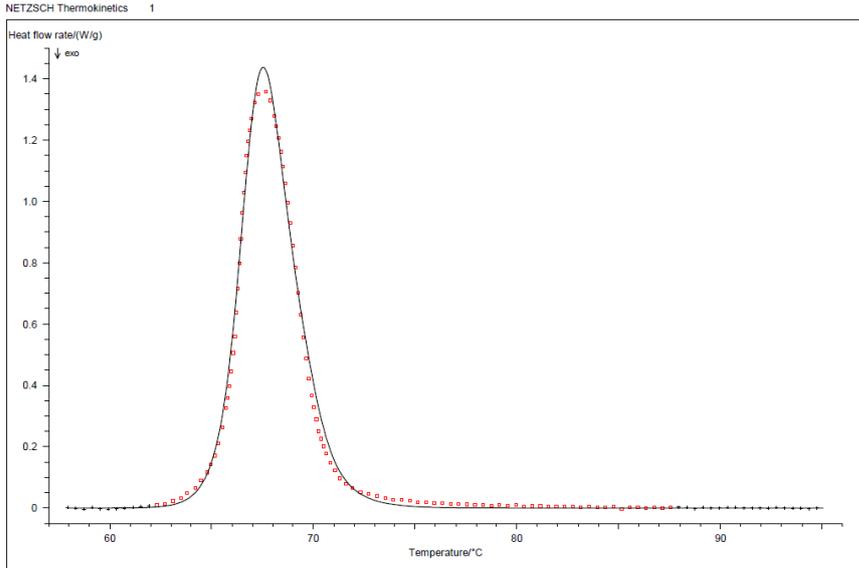
NETZSCH Thermokinetics

Date/Time: 02.10.2016 at 18:20

Project: 1
Model 1: n-th order with autocatalysis by B

A —1→B

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP320 08.05.2016 18:14:53/Segm.S2/3		
Transfer Corr.	204 F1.kcr			
Min. Temp/°C:	57.9281	Min. Time/min:		0.0
Max. Temp/°C:	95.0449	Max. Time/min:		6.2092
Heating rate/(K/min):	5.978	Sampling time/s:		1.004
Sample mass/mg:	3.510			
Base line type:	tangent area prop.	LeftPts: 40		RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	100.0134	198.6281				0.5749
1	E1 kJ/mol	661.5171	1302.1281			+	4.1965
2	React.ord. 1	1.8310	2.6760			+	9.4951E-2
3	log Kcat 1	0.4500	0.2779				0.2501
4	Area 1/(J/g)	50.0664	50.0664				constant

STATISTICS

Least squares:	2.22262	Number of cycles:	36
Mean of residues:	7.72967E-2	Max.No of cycles:	50
Correlation coefficient:	0.997662	Rel. precision:	0.001000
Durbin-Watson Value:	0.069	t-critical(0.95;250):	1.961
Durbin-Watson Factor:	3.835		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.23	250	Cn B					
1	s:	2.34	1.24	228	Bna					
2	s:	2.47	1.24	229	Fn					
3	s:	2.99	1.24	230	B1					
4	s:	3.04	1.24	229	C1 B					
5	s:	3.72	1.24	230	F2					
6	s:	9.91	1.24	229	An					
7	s:	12.53	1.24	230	A2					
8	s:	17.02	1.24	230	F1					
9	s:	30.67	1.24	230	R3					
10	s:	36.16	1.24	230	D1F					
11	s:	38.62	1.24	230	D3F					
12	s:	39.69	1.24	230	D3					
13	s:	41.53	1.24	230	R2					
14	s:	58.88	1.24	230	D4					
15	s:	73.48	1.24	230	D2					
16	s:	112.04	1.24	230	D1					
17	s:	535.36	1.24	230	A3					

Sample 12 / cycle 4 / CnB
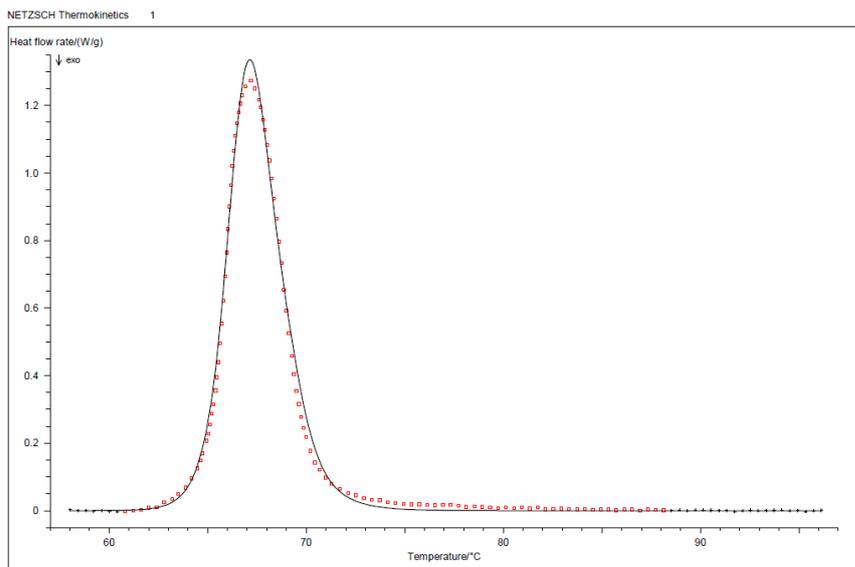
NETZSCH Thermokinetics

Date/Time: 02.10.2016 at 18:21

Project: 1
Model 1: n-th order with autocatalysis by B

$A \xrightarrow{1} B$

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 08.05.2016 18:56:23/Segm.S2/3
Transfer Corr.:	204_F1.kcr		
Min. Temp/°C:	58.0196	Min. Time/min:	0.0
Max. Temp°C:	96.1368	Max. Time/min:	6.3765
Heating rate/(K/min):	5.978	Sampling time/s:	1.004
Sample mass/mg:	3.590		
Base line type:	tangent area prop.	LeftPts: 40	RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	113.1644	190.2537				0.4485
1	E1 kJ/mol	746.0846	1246.1773			+	3.3226
2	React.ord. 1	2.0548	2.6422			+	8.3800E-2
3	log Kcat 1	0.4500	0.2699				0.2246
4	Area 1/(J/g)	47.4723	47.4723				constant

STATISTICS

Least squares:	1.75318	Number of cycles:	38
Mean of residues:	6.77457E-2	Max.No of cycles:	50
Correlation coefficient:	0.997867	Rel. precision:	0.001000
Durbin-Watson Value:	0.059	t-critical(0.95;272):	1.960
Durbin-Watson Factor:	4.137		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.22	272	Cn B					
1	s:	3.22	1.24	228	Bna					
2	s:	3.41	1.24	229	Fn					
3	s:	4.12	1.23	230	B1					
4	s:	4.20	1.24	229	C1 B					
5	s:	5.13	1.23	230	F2					
6	s:	13.67	1.24	229	An					
7	s:	17.28	1.23	230	A2					
8	s:	23.48	1.23	230	F1					
9	s:	42.30	1.23	230	R3					
10	s:	49.87	1.23	230	D1F					
11	s:	53.28	1.23	230	D3F					
12	s:	54.75	1.23	230	D3					
13	s:	57.29	1.23	230	R2					
14	s:	81.21	1.23	230	D4					
15	s:	101.36	1.23	230	D2					
16	s:	154.54	1.23	230	D1					
17	s:	738.44	1.23	230	A3					

Sample 12 / cycle 5 / CnB

NETZSCH Thermokinetics   1

Heat flow rate/(W/g)

| | Temperature/°C |
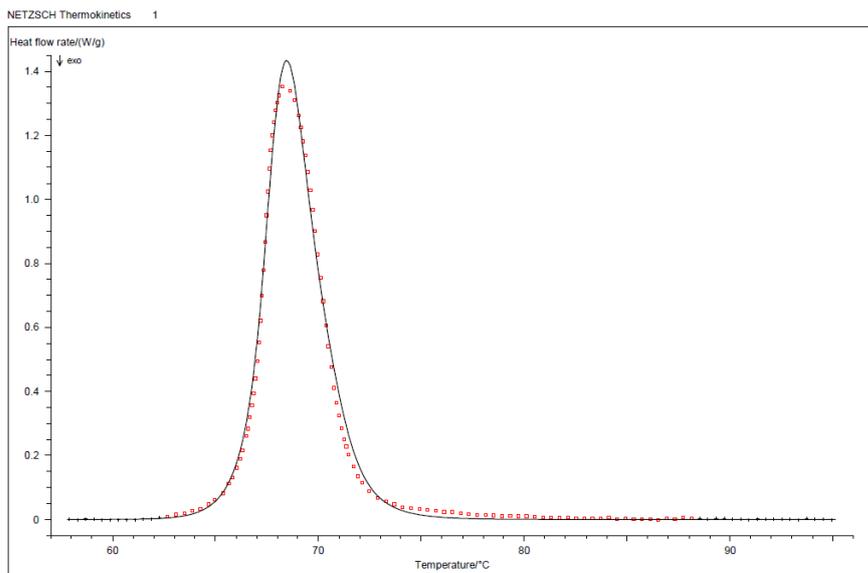
NETZSCH Thermokinetics   Date/Time: 02.10.2016 at 18:22
Project: 1
Model   1: n-th order with autocatalysis by B   A—1→B

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP320 10.05.2016 11:06:30/Segm.S2/3		
Transfer Corr:	204_F1.kcr			
Min. Temp/°C:	57.8882	Min. Time/min:		0.0
Max. Temp°C:	95.1155	Max. Time/min:		6.2262
Heating rate/(K/min):	5.979	Sampling time/s:		1.004
Sample mass/mg:	3.590			
Base line type:	tangent area prop.	LeftPts: 40		RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	118.6294	151.5184				0.1179
1	E1 kJ/mol	784.6287	1000.0203			+	1.0079
2	React.ord. 1	2.0816	2.4330			+	5.7120E-2
3	log Kcat 1	0.4500	0.7524				8.4728E-2
4	Area 1/(J/g)	49.9103	49.9103				constant

STATISTICS

Least squares:	2.24752	Number of cycles:		40
Mean of residues:	7.76243E-2	Max.No of cycles:		50
Correlation coefficient:	0.997581	Rel. precision:		0.001000
Durbin-Watson Value:	0.068	t-critical(0.95;254):		1.960
Durbin-Watson Factor:	3.874			

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.23	254	Cn B					
1	s:	2.35	1.24	228	Bna					
2	s:	2.49	1.24	229	Fn					
3	s:	3.00	1.24	230	B1					
4	s:	3.06	1.24	229	C1 B					
5	s:	3.73	1.24	230	F2					
6	s:	9.96	1.24	229	An					
7	s:	12.59	1.24	230	A2					
8	s:	17.10	1.24	230	F1					
9	s:	30.81	1.24	230	R3					
10	s:	36.33	1.24	230	D1F					
11	s:	38.81	1.24	230	D3F					
12	s:	39.88	1.24	230	D3					
13	s:	41.73	1.24	230	R2					
14	s:	59.16	1.24	230	D4					
15	s:	73.83	1.24	230	D2					
16	s:	112.57	1.24	230	D1					
17	s:	537.90	1.24	230	A3					
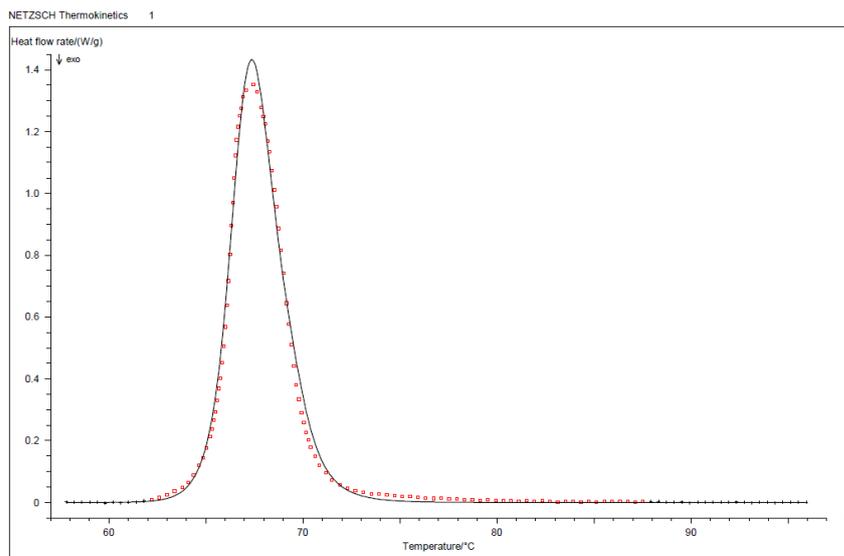
NETZSCH Thermokinetics

Date/Time: 02.10.2016 at 18:24

Project: 1
Model 1: n-th order with autocatalysis by B

$A \overset{1}{\longrightarrow} B$

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 10.05.2016 12:19:04/Segm.S2/3	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	57.8150	Min. Time/min:	0.0
Max. Temp°C:	95.9355	Max. Time/min:	6.3773
Heating rate/(K/min):	5.978	Sampling time/s:	1.004
Sample mass/mg:	3.590		
Base line type:	tangent area prop.	LeftPts: 40	RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	106.8482	191.2357				0.3828
1	E1 kJ/mol	705.5683	1253.7668			+	2.8795
2	React.ord. 1	1.9044	2.6390			+	8.1459E-2
3	log Kcat 1	0.4500	0.4068				0.1806
4	Area 1/(J/g)	49.1861	49.1861				constant

STATISTICS

Least squares:	2.42868	Number of cycles:	46
Mean of residues:	7.97358E-2	Max.No of cycles:	50
Correlation coefficient:	0.997326	Rel. precision:	0.001000
Durbin-Watson Value:	0.083	t-critical(0.95;251):	1.961
Durbin-Watson Factor:	3.507		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.23	251	Cn B					
1	s:	2.15	1.24	228	Bna					
2	s:	2.27	1.24	229	Fn					
3	s:	2.74	1.24	230	B1					
4	s:	2.80	1.24	229	C1 B					
5	s:	3.42	1.24	230	F2					
6	s:	9.11	1.24	229	An					
7	s:	11.51	1.24	230	A2					
8	s:	15.64	1.24	230	F1					
9	s:	28.18	1.24	230	R3					
10	s:	33.22	1.24	230	D1F					
11	s:	35.49	1.24	230	D3F					
12	s:	36.47	1.24	230	D3					
13	s:	38.16	1.24	230	R2					
14	s:	54.10	1.24	230	D4					
15	s:	67.52	1.24	230	D2					
16	s:	102.94	1.24	230	D1					
17	s:	491.90	1.24	230	A3					

Sample 12 / cycle 7 / CnB
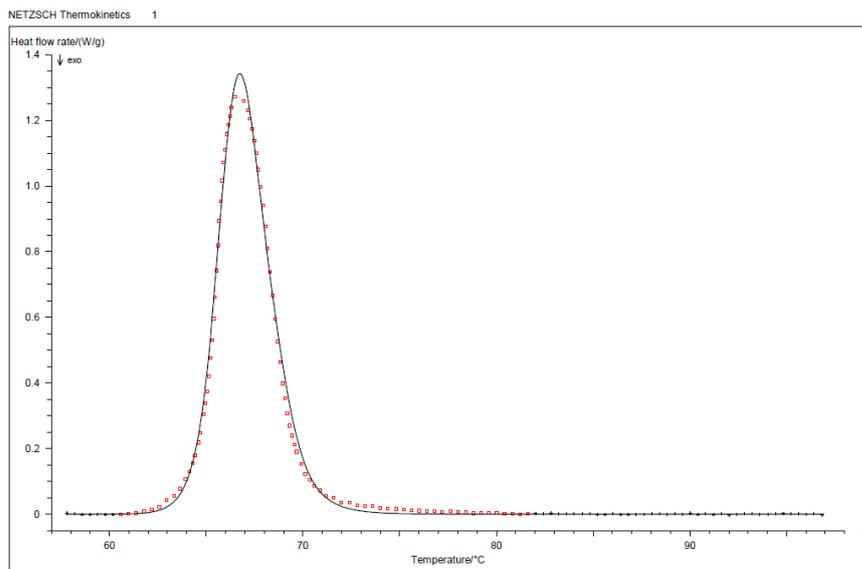
NETZSCH Thermokinetics

Date/Time: 02.10.2016 at 18:25

Project: 1
Model 1: n-th order with autocatalysis by B

A —1→ B

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 10.05.2016 13:07:36/Segm.S2/3
Transfer Corr:	204_F1.kcr		
Min. Temp°C:	57.8006	Min. Time/min:	0.0
Max. Temp°C:	96.9202	Max. Time/min:	6.5456
Heating rate/(K/min):	5.976	Sampling time/s:	1.004
Sample mass/mg:	3.590		
Base line type:	tangent area prop.	LeftPts: 40	RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	96.0626	217.3859				1.3840
1	E1 kJ/mol	634.3342	1420.2485			+	9.7384
2	React.ord. 1	1.7644	2.6963			+	0.1934
3	log Kcat 1	0.4500	-3.4406E-2				0.7069
4	Area 1/(J/g)	46.5225	46.5225				constant

STATISTICS

Least squares:	1.46878	Number of cycles:	28
Mean of residues:	6.12118E-2	Max.No of cycles:	50
Correlation coefficient:	0.998079	Rel. precision:	0.001000
Durbin-Watson Value:	0.074	t-critical(0.95;213):	1.962
Durbin-Watson Factor:	3.713		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.25	213	Cn B					
1	s:	3.01	1.25	228	Bna					
2	s:	3.19	1.25	229	Fn					
3	s:	3.85	1.25	230	B1					
4	s:	3.92	1.25	229	C1 B					
5	s:	4.79	1.25	230	F2					
6	s:	12.78	1.25	229	An					
7	s:	16.15	1.25	230	A2					
8	s:	21.95	1.25	230	F1					
9	s:	39.54	1.25	230	R3					
10	s:	46.62	1.25	230	D1F					
11	s:	49.80	1.25	230	D3F					
12	s:	51.17	1.25	230	D3					
13	s:	53.55	1.25	230	R2					
14	s:	75.91	1.25	230	D4					
15	s:	94.74	1.25	230	D2					
16	s:	144.45	1.25	230	D1					
17	s:	690.24	1.25	230	A3					

Sample 12 / cycle 8 / CnB
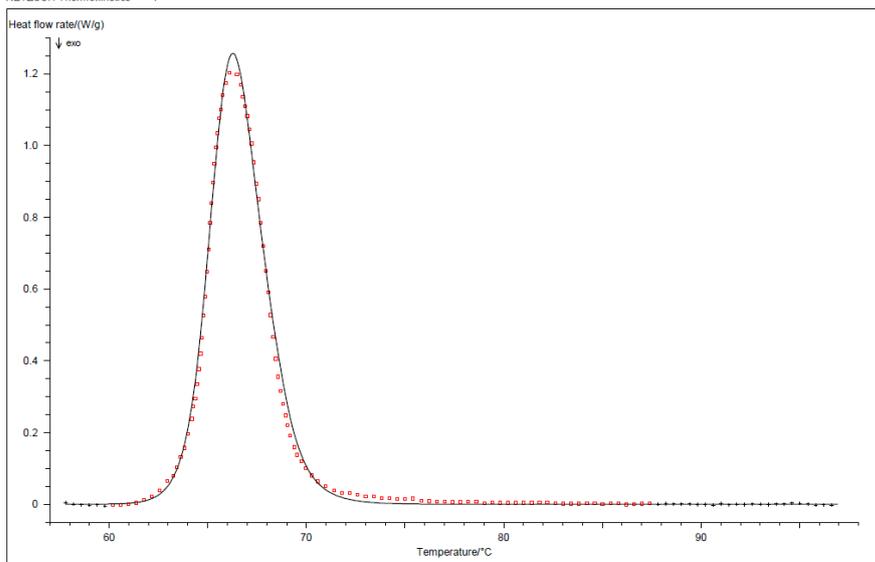
NETZSCH Thermokinetics   Date/Time: 02.10.2016 at 18:26
Project: 1
Model   1: n-th order with autocatalysis by B   A — 1 → B

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 10.05.2016 13:49:34/Segm.S2/3	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	57.8028	Min. Time/min:	0.0
Max. Temp°C:	96.9197	Max. Time/min:	6.5454
Heating rate/(K/min):	5.976	Sampling time/s:	1.004
Sample mass/mg:	3.590		
Base line type:	tangent area prop.	LeftPts: 40	RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	100.6290	208.9708				1.2333
1	E1 kJ/mol	663.0398	1363.6365			+	8.6475
2	React.ord. 1	1.8819	2.6377			+	0.1816
3	log Kcat 1	0.4500	-0.1521				0.7660
4	Area 1/(J/g)	44.8269	44.8269				constant

STATISTICS

Least squares:	1.17668	Number of cycles:	38
Mean of residues:	5.47880E-2	Max.No of cycles:	50
Correlation coefficient:	0.998380	Rel. precision:	0.001000
Durbin-Watson Value:	0.083	t-critical(0.95;271):	1.960
Durbin-Watson Factor:	3.517		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.22	271	Cn B					
1	s:	4.78	1.24	228	Bna					
2	s:	5.07	1.24	229	Fn					
3	s:	6.12	1.23	230	B1					
4	s:	6.23	1.24	229	C1 B					
5	s:	7.61	1.23	230	F2					
6	s:	20.29	1.24	229	An					
7	s:	25.65	1.23	230	A2					
8	s:	34.86	1.23	230	F1					
9	s:	62.79	1.23	230	R3					
10	s:	74.03	1.23	230	D1F					
11	s:	79.09	1.23	230	D3F					
12	s:	81.27	1.23	230	D3					
13	s:	85.04	1.23	230	R2					
14	s:	120.55	1.23	230	D4					
15	s:	150.46	1.23	230	D2					
16	s:	229.41	1.23	230	D1					
17	s:	1096.19	1.23	230	A3					
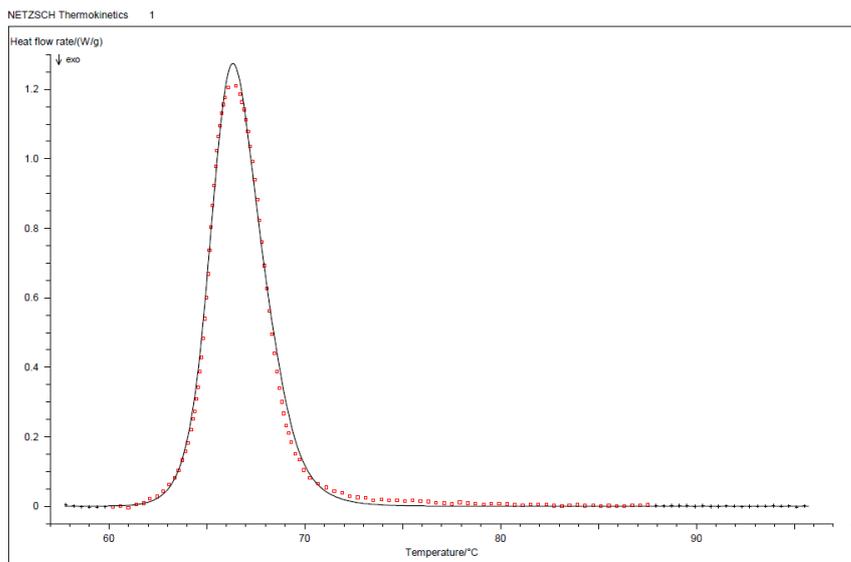
NETZSCH Thermokinetics

Date/Time: 02.10.2016 at 18:28

Project: 1
Model 1: n-th order with autocatalysis by B

$$A \xrightarrow{\ 1\ } B$$

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 10.05.2016 14:30:57/Segm.S2/3
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	57.8058	Min. Time/min:	0.0
Max. Temp°C:	95.7260	Max. Time/min:	6.3420
Heating rate/(K/min):	5.979	Sampling time/s:	1.004
Sample mass/mg:	3.590		
Base line type:	tangent area prop.	LeftPts: 40	RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	101.4546	204.7274				0.9988
1	E1 kJ/mol	668.4994	1336.5919			+	7.0905
2	React.ord. 1	1.9040	2.6810			+	0.1450
3	log Kcat 1	0.4500	3.1726E-2				0.5059
4	Area 1/(J/g)	45.2092	45.2092				constant

STATISTICS

Least squares:	1.38530	Number of cycles:	34
Mean of residues:	6.03783E-2	Max.No of cycles:	50
Correlation coefficient:	0.998176	Rel. precision:	0.001000
Durbin-Watson Value:	0.065	t-critical(0.95;272):	1.960
Durbin-Watson Factor:	3.949		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.22	272	Cn B					
1	s:	4.08	1.24	228	Bna					
2	s:	4.32	1.24	229	Fn					
3	s:	5.21	1.23	230	B1					
4	s:	5.31	1.24	229	C1 B					
5	s:	6.49	1.23	230	F2					
6	s:	17.30	1.24	229	An					
7	s:	21.87	1.23	230	A2					
8	s:	29.72	1.23	230	F1					
9	s:	53.53	1.23	230	R3					
10	s:	63.11	1.23	230	D1F					
11	s:	67.42	1.23	230	D3F					
12	s:	69.29	1.23	230	D3					
13	s:	72.50	1.23	230	R2					
14	s:	102.78	1.23	230	D4					
15	s:	128.27	1.23	230	D2					
16	s:	195.58	1.23	230	D1					
17	s:	934.54	1.23	230	A3					

Sample 13 / cycle 1 / CnB

NETZSCH Thermokinetics
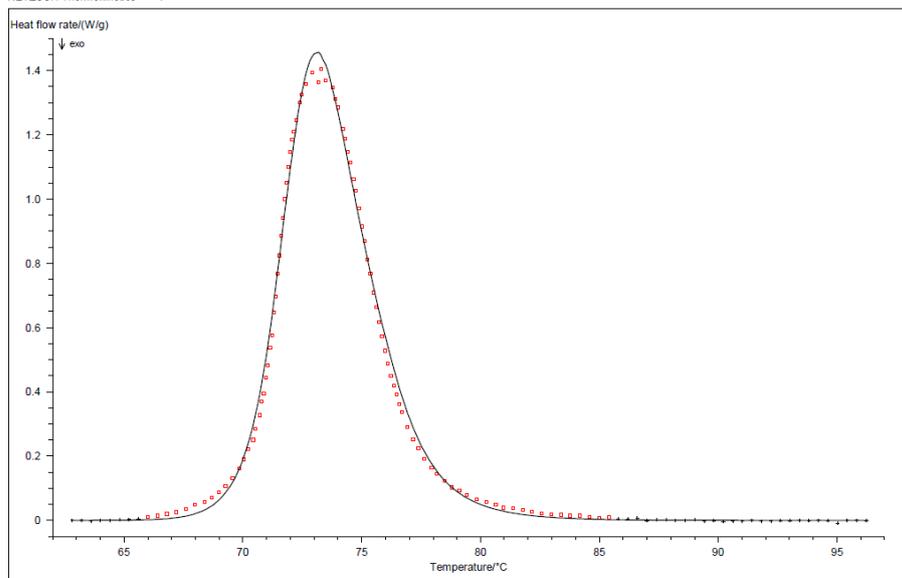
Date/Time: 02.10.2016 at 14:48

Project: 1
Model   1: n-th order with autocatalysis by B

$A \xrightarrow{1} B$

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 27.06.2016 15:34:13/Segm.S1/3	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	62.8057	Min. Time/min:	0.0
Max. Temp°C:	96.3237	Max. Time/min:	3.7324
Heating rate/(K/min):	8.980	Sampling time/s:	0.670
Sample mass/mg:	4.100		
Base line type:		LeftPts: 30	RightPts: 30

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	65.9868	163.1361				1.3743E-2
1	E1 kJ/mol	446.8769	1087.3034			+	0.3219
2	React.ord. 1	1.7090	2.9823			+	8.8537E-2
3	log Kcat 1	0.4500	0.1307				0.1023
4	Area 1/(J/g)	46.7341	46.7341				constant

STATISTICS

Least squares:	2.12728	Number of cycles:	21
Mean of residues:	7.96875E-2	Max.No of cycles:	50
Correlation coefficient:	0.998245	Rel. precision:	0.001000
Durbin-Watson Value:	0.109	t-critical(0.95;194):	1.963
Durbin-Watson Factor:	3.066		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.27	194	Cn B					
1	s:	1.23	1.27	195	Fn					
2	s:	1.40	1.27	195	C1 B					
3	s:	3.53	1.27	196	F2					
4	s:	7.98	1.27	195	An					
5	s:	13.22	1.27	196	A2					
6	s:	17.59	1.27	196	F1					
7	s:	20.84	1.27	196	A3					
8	s:	30.61	1.27	196	R3					
9	s:	33.50	1.27	196	D1F					
10	s:	36.50	1.27	196	D3F					
11	s:	37.73	1.27	196	D3					
12	s:	40.50	1.27	196	R2					
13	s:	54.64	1.27	196	D4					
14	s:	68.70	1.27	196	D2					
15	s:	100.64	1.27	196	D1					

Sample 13 / cycle 2 / CnB

NETZSCH Thermokinetics
Project: 1
Model   1: n-th order with autocatalysis by B

Date/Time: 02.10.2016 at 14:54

$A-1\rightarrow B$

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 27.06.2016 16:05:07/Segm.S1/3
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	58.2038	Min. Time/min:	0.0
Max. Temp°C:	88.5867	Max. Time/min:	3.4067
Heating rate/(K/min):	8.918	Sampling time/s:	0.670
Sample mass/mg:	4.100		
Base line type:		LeftPts: 102	RightPts: 100

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	60.6060	162.1685				1.5287E-2
1	E1 kJ/mol	409.7811	1076.3667			+	0.3501
2	React.ord. 1	1.3847	2.4198			+	0.1018
3	log Kcat 1	0.4500	-0.1509				0.1351
4	Area 1/(J/g)	48.2167	48.2167				constant

STATISTICS

Least squares:	2.22038	Number of cycles:	23
Mean of residues:	8.51830E-2	Max.No of cycles:	50
Correlation coefficient:	0.998626	Rel. precision:	0.001000
Durbin-Watson Value:	0.032	t-critical(0.95;193):	1.963
Durbin-Watson Factor:	5.599		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.27	193	Cn B					
1	s:	1.10	1.27	194	Fn					
2	s:	1.23	1.27	195	B1					
3	s:	1.29	1.27	194	C1 B					
4	s:	1.66	1.27	195	F2					
5	s:	6.38	1.27	193	Bna					
6	s:	7.51	1.27	194	An					
7	s:	9.90	1.27	195	A2					
8	s:	14.16	1.27	195	F1					
9	s:	17.58	1.27	195	A3					
10	s:	28.27	1.27	195	R3					
11	s:	33.04	1.27	195	D1F					
12	s:	35.90	1.27	195	D3F					
13	s:	37.15	1.27	195	D3					
14	s:	39.59	1.27	195	R2					
15	s:	57.00	1.27	195	D4					
16	s:	74.62	1.27	195	D2					
17	s:	116.62	1.27	195	D1					

Sample 13 / cycle 3 / CnB
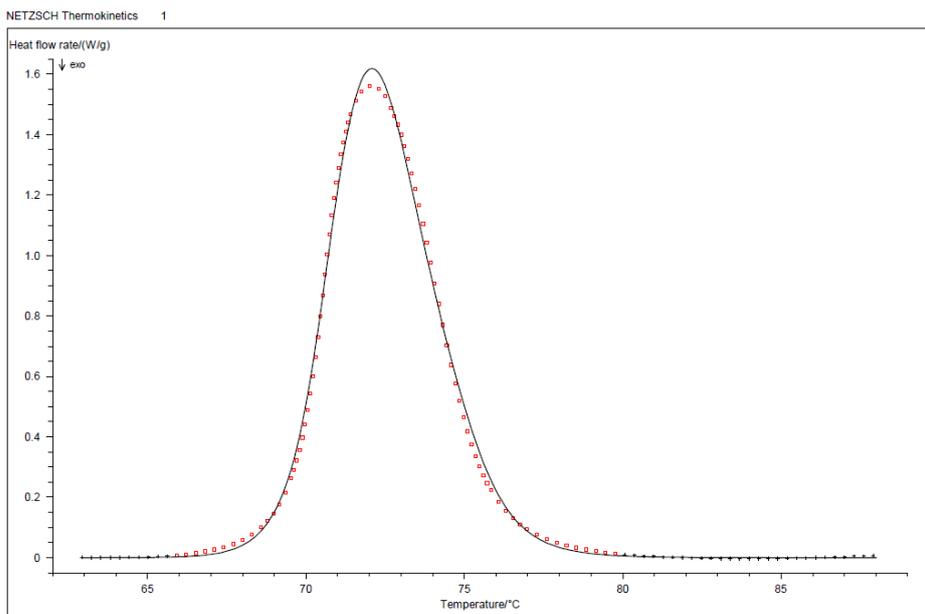
NETZSCH Thermokinetics

Date/Time: 02.10.2016 at 15:07

Project: 1
Model   1: Prout-Tompkins n-th order, a autocat   A −1→ B

Start evaluation:		0.00050	Measurement type:		DSC
Fine evaluation:		0.99950			
SCAN 1	Identity:		OP320 27.06.2016 17:55:36/Segm.S1/3		
Transfer Corr:		204_F1.kcr			
Min. Temp/°C:		62.9208	Min. Time/min:		0.0
Max. Temp°C:		88.0067	Max. Time/min:		2.7997
Heating rate/(K/min):		8.960	Sampling time/s:		0.672
Sample mass/mg:		4.100			
Base line type:		tangent area prop.	LeftPts: 20		RightPts: 70

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	25.0106	151.0600				2.3748E-2
1	E1 kJ/mol	172.2698	1003.1475			+	0.1558
2	React.ord. 1	0.8687	2.1999			+	9.3763E-2
3	Exponent a1	0.5205	0.2204			+	2.7768E-2
4	Area 1/(J/g)	46.8653	46.8653				constant

STATISTICS

Least squares:	2.21469	Number of cycles:	17
Mean of residues:	9.39332E-2	Max.No of cycles:	50
Correlation coefficient:	0.998691	Rel. precision:	0.001000
Durbin-Watson Value:	0.044	t-critical(0.95;138):	1.968
Durbin-Watson Factor:	4.801		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.33	138	Bna					
1	s:	1.04	1.33	139	Fn					
2	s:	2.08	1.33	138	Cn B					
3	s:	2.77	1.33	139	C1 B					
4	s:	2.83	1.32	140	F2					
5	s:	4.73	1.32	140	B1					
6	s:	7.26	1.33	139	An					
7	s:	14.08	1.32	140	A2					
8	s:	21.08	1.32	140	F1					
9	s:	39.67	1.32	140	R3					
10	s:	47.67	1.32	140	D1F					
11	s:	50.94	1.32	140	D3F					
12	s:	52.21	1.32	140	D3					
13	s:	54.24	1.32	140	R2					
14	s:	60.29	1.32	140	A3					
15	s:	78.17	1.32	140	D4					
16	s:	97.99	1.32	140	D2					
17	s:	145.20	1.32	140	D1					

Sample 13 / cycle 4 / CnB
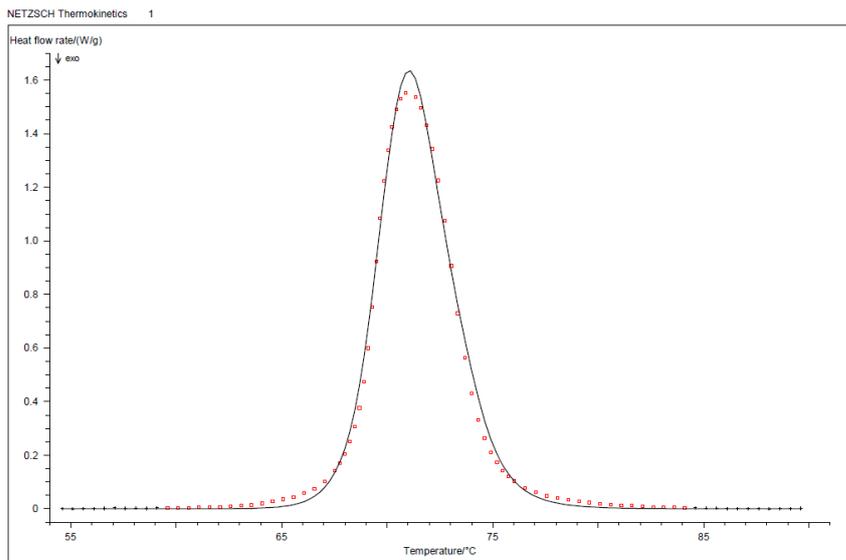
NETZSCH Thermokinetics

Date/Time: 02.10.2016 at 15:11

Project: 1
Model 1: n-th order with autocatalysis by B

$A \xrightarrow{1} B$

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 27.06.2016 18:34:46/Segm.S1/3	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	54.6004	Min. Time/min:	0.0
Max. Temp°C:	89.6176	Max. Time/min:	3.9143
Heating rate/(K/min):	8.946	Sampling time/s:	1.678
Sample mass/mg:	4.100		
Base line type:	tangent area prop.	LeftPts: 5	RightPts: 5

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	71.7332	163.2366				2.5427E-2
1	E1 kJ/mol	481.8720	1081.2562			+	0.5760
2	React.ord. 1	1.5971	2.5488			+	0.1805
3	log Kcat 1	0.4500	-4.7244E-3				0.1813
4	Area 1/(J/g)	49.1561	49.1561				constant

STATISTICS

Least squares:	3.61527	Number of cycles:	21
Mean of residues:	0.16013	Max.No of cycles:	50
Correlation coefficient:	0.997697	Rel. precision:	0.001000
Durbin-Watson Value:	0.195	t-critical(0.95;96):	1.976
Durbin-Watson Factor:	2.322		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.40	96	Cn B					
1	s:	1.08	1.40	97	Fn					
2	s:	1.10	1.40	98	B1					
3	s:	1.19	1.40	97	C1 B					
4	s:	1.58	1.40	98	F2					
5	s:	5.09	1.40	97	An					
6	s:	6.05	1.40	98	A2					
7	s:	8.50	1.40	98	F1					
8	s:	15.90	1.40	98	A3					
9	s:	15.99	1.40	98	R3					
10	s:	18.54	1.40	98	D1F					
11	s:	20.30	1.40	98	D3F					
12	s:	20.96	1.40	98	D3					
13	s:	22.29	1.40	98	R2					
14	s:	31.40	1.40	98	D4					
15	s:	45.12	1.40	98	D2					
16	s:	62.61	1.40	98	D1					
17	s:	1064.75	1.40	96	Bna					
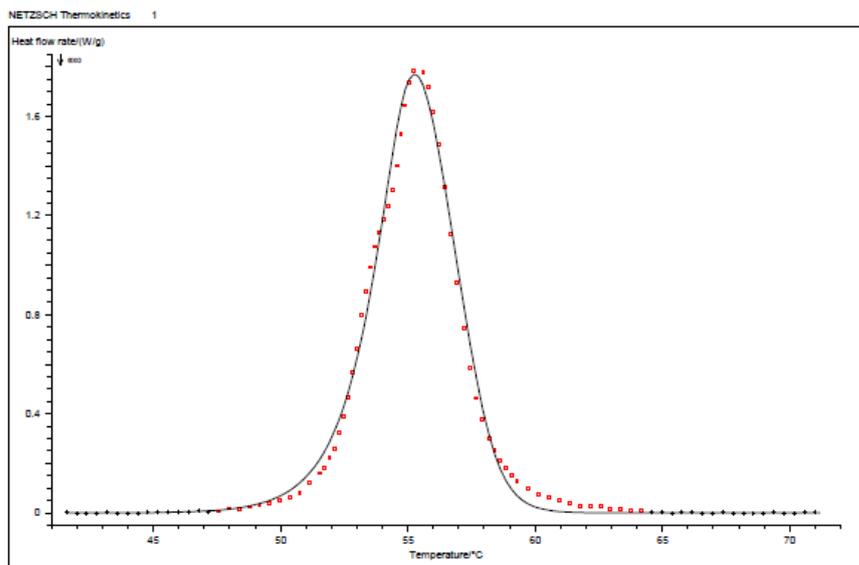
NETZSCH Thermokinetics

Project: 1
Model 1: n-th order with autocatalysis by B

A — 1 → B

Date/Time: 04.10.2016 at 14:08

Start evaluation:	0.00050	Measurement type: DSC
Fine evaluation:	0.99950	
SCAN 1 Identity:		OP320 08.04.2016 12:36:46/Segm.S1/3
Transfer Corr:	204_F1.kcr	
Min. Temp/°C:	41.5858	Min. Time/min: 0.0
Max. Temp°C:	71.1736	Max. Time/min: 3.3078
Heating rate/(K/min):	8.945	Sampling time/s: 1.341
Sample mass/mg:	2.800	
Base line type:	tangent area prop.	LeftPts: 25 RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	77.9509	100.9311				4.9770E-2
1	E1 kJ/mol	498.9482	642.0715			+	0.9274
2	React.ord. 1	1.3512	1.5018			+	0.4545
3	log Kcat 1	0.4500	0.2302				6.3181E-2
4	Area 1/(J/g)	49.7760	49.7760				constant

STATISTICS

Least squares:	7.51554	Number of cycles:	19
Mean of residues:	0.22459	Max.No of cycles:	50
Correlation coefficient:	0.995799	Rel. precision:	0.001000
Durbin-Watson Value:	0.164	t-critical(0.95;82):	1.980
Durbin-Watson Factor:	2.525		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.44	82	Cn B					
1	s:	1.10	1.44	83	C1 B					
2	s:	1.27	1.44	83	Fn					
3	s:	1.53	1.44	83	An					
4	s:	1.54	1.44	84	B1					
5	s:	1.63	1.44	84	A3					
6	s:	1.78	1.44	84	A2					
7	s:	1.95	1.44	84	F2					
8	s:	2.25	1.44	84	F1					
9	s:	5.28	1.44	84	R3					
10	s:	5.52	1.44	84	D1F					
11	s:	5.96	1.44	84	D3F					
12	s:	6.55	1.44	84	D3					
13	s:	8.19	1.44	84	R2					
14	s:	11.80	1.44	84	D4					
15	s:	16.35	1.44	84	D2					
16	s:	29.83	1.44	84	D1					

Sample 15 / cycle 3 / CnB

NETZSCH Thermokinetics   1
Heat flow rate/(W/g)
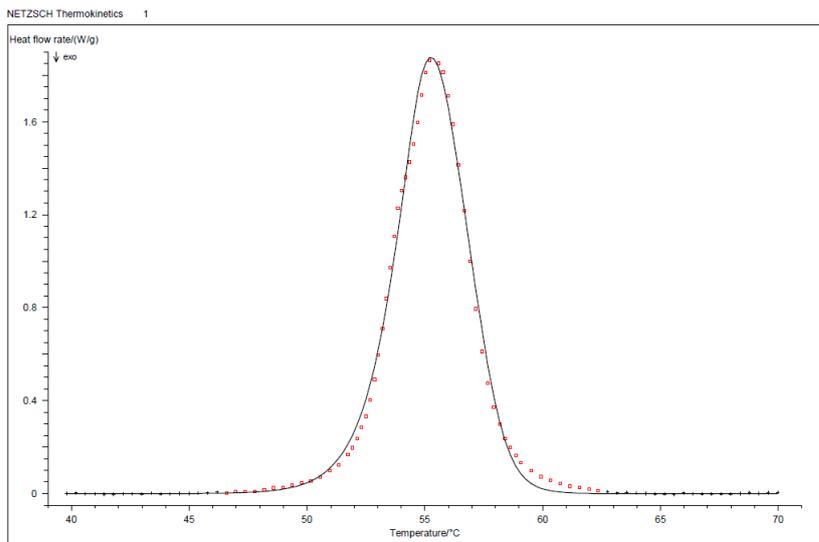
NETZSCH Thermokinetics   Date/Time: 04.10.2016 at 14:06
Project: 1
Model   1: n-th order with autocatalysis by B   A — 1→ B

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP320 08.04.2016 13:16:26/Segm.S1/3		
Transfer Corr:	204_F1.kcr			
Min. Temp/°C:	39.7895	Min. Time/min:		0.0
Max. Temp°C:	69.9776	Max. Time/min:		3.3746
Heating rate/(K/min):	8.946	Sampling time/s:		1.341
Sample mass/mg:	2.800			
Base line type:	tangent area prop.	LeftPts: 30		RightPts: 30

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	55.7714	121.6263				6.7202E-2
1	E1 kJ/mol	360.0400	771.2089			+	0.9924
2	React.ord. 1	1.0651	1.5842			+	0.1768
3	log Kcat 1	0.4500	-4.6182E-2				0.3075
4	Area 1/(J/g)	50.8102	50.8102				constant

STATISTICS

Least squares:	5.13259	Number of cycles:	20
Mean of residues:	0.18376	Max.No of cycles:	50
Correlation coefficient:	0.997313	Rel. precision:	0.001000
Durbin-Watson Value:	0.197	t-critical(0.95;77):	1.982
Durbin-Watson Factor:	2.312		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.46	77	Cn B					
1	s:	1.16	1.46	78	Fn					
2	s:	1.28	1.46	78	C1 B					
3	s:	1.69	1.46	79	B1					
4	s:	1.84	1.46	79	F2					
5	s:	2.12	1.46	78	An					
6	s:	2.14	1.46	79	A3					
7	s:	2.33	1.46	79	A2					
8	s:	3.13	1.46	79	F1					
9	s:	8.27	1.46	79	R3					
10	s:	9.33	1.46	79	D1F					
11	s:	9.86	1.46	79	D3F					
12	s:	10.57	1.46	79	D3					
13	s:	12.90	1.46	79	R2					
14	s:	19.06	1.46	79	D4					
15	s:	25.43	1.46	79	D2					
16	s:	47.72	1.46	79	D1					

Sample 15 / cycle 4 / CnB
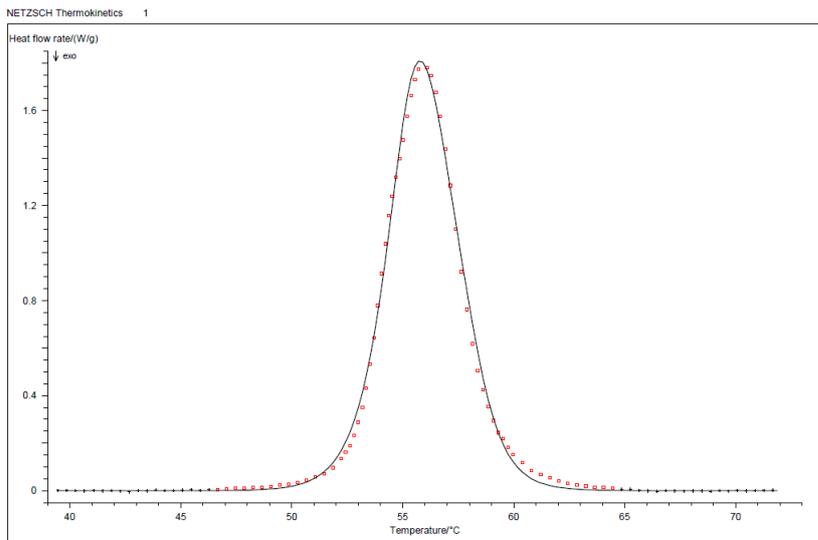
NETZSCH Thermokinetics

Date/Time: 04.10.2016 at 14:04

Project: 1
Model   1: n-th order with autocatalysis by B   A —1→B

Start evaluation:		0.00050	Measurement type:		DSC
Fine evaluation:		0.99950			
SCAN 1	Identity:		OP320 11.04.2016 14:04:20/Segm.S1/1		
Transfer Corr:		204 F1.kcr			
Min. Temp/°C:		39.4751	Min. Time/min:		0.0
Max. Temp°C:		71.8624	Max. Time/min:		3.6230
Heating rate/(K/min):		8.939	Sampling time/s:		1.342
Sample mass/mg:		2.800			
Base line type:		tangent area prop.	LeftPts: 30		RightPts: 30

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	83.2931	136.8992				2.9766E-2
1	E1 kJ/mol	533.0454	868.1465			+	0.6075
2	React.ord. 1	1.6039	2.0037			+	0.2204
3	log Kcat 1	0.4500	-6.1090E-2				0.1516
4	Area 1/(J/g)	51.1448	51.1448				constant

STATISTICS

Least squares:	3.56840	Number of cycles:	21
Mean of residues:	0.14796	Max.No of cycles:	50
Correlation coefficient:	0.997992	Rel. precision:	0.001000
Durbin-Watson Value:	0.175	t-critical(0.95;86):	1.979
Durbin-Watson Factor:	2.448		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.43	86	Cn B					
1	s:	1.16	1.43	88	F2					
2	s:	1.17	1.43	87	Fn					
3	s:	1.19	1.43	88	B1					
4	s:	1.24	1.43	87	C1 B					
5	s:	5.21	1.43	87	An					
6	s:	5.26	1.43	88	A3					
7	s:	5.64	1.43	88	A2					
8	s:	7.27	1.43	88	F1					
9	s:	15.93	1.43	88	R3					
10	s:	17.55	1.43	88	D1F					
11	s:	18.68	1.43	88	D3F					
12	s:	19.63	1.43	88	D3					
13	s:	23.68	1.43	88	R2					
14	s:	31.70	1.43	88	D4					
15	s:	43.28	1.43	88	D2					
16	s:	70.70	1.43	88	D1					

Sample 15 / cycle 5 / CnB
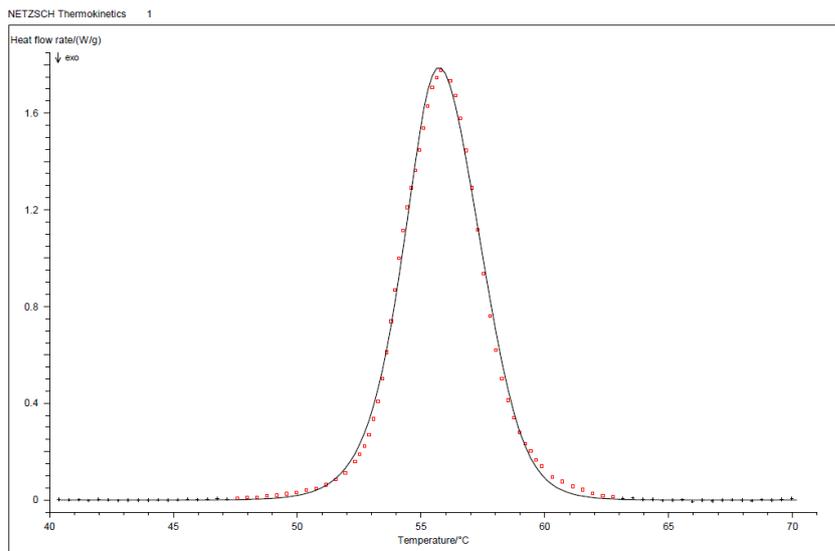
NETZSCH Thermokinetics

Date/Time: 04.10.2016 at 14:02

Project: 1
Model 1: n-th order with autocatalysis by B

$A \xrightarrow{1} B$

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 12.04.2016 10:38:01/Segm.S1/1
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	40.3786	Min. Time/min:	0.0
Max. Temp°C:	70.1669	Max. Time/min:	3.3347
Heating rate/(K/min):	8.933	Sampling time/s:	1.343
Sample mass/mg:	2.800		
Base line type:	tangent area prop.	LeftPts: 30	RightPts: 30

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	69.9847	139.1724				0.2408
1	E1 kJ/mol	449.5754	882.1656			+	2.4608
2	React.ord. 1	1.3663	1.9223			+	0.1003
3	log Kcat 1	0.4500	-0.1881				0.9867
4	Area 1/(J/g)	49.8439	49.8439				constant

STATISTICS

Least squares:	3.08812	Number of cycles:	21
Mean of residues:	0.14348	Max.No of cycles:	50
Correlation coefficient:	0.998252	Rel. precision:	0.001000
Durbin-Watson Value:	0.184	t-critical(0.95;75):	1.983
Durbin-Watson Factor:	2.386		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.47	75	Cn B					
1	s:	1.13	1.47	76	Fn					
2	s:	1.17	1.46	77	F2					
3	s:	1.37	1.46	77	B1					
4	s:	1.42	1.47	76	C1 B					
5	s:	5.39	1.47	76	An					
6	s:	5.47	1.46	77	A3					
7	s:	5.90	1.46	77	A2					
8	s:	7.75	1.46	77	F1					
9	s:	18.00	1.46	77	R3					
10	s:	20.16	1.46	77	D1F					
11	s:	21.30	1.46	77	D3F					
12	s:	22.36	1.46	77	D3					
13	s:	27.25	1.46	77	R2					
14	s:	36.96	1.46	77	D4					
15	s:	49.87	1.46	77	D2					
16	s:	83.58	1.46	77	D1					

Sample 15 / cycle 6 / CnB

NETZSCH Thermokinetics
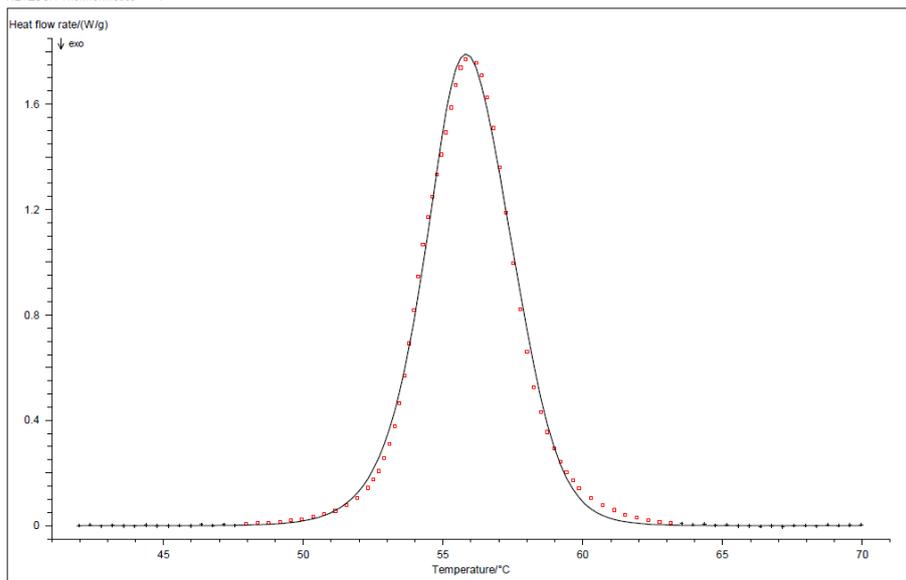
Date/Time: 04.10.2016 at 14:00

Project: 1
Model   1: n-th order with autocatalysis by B $A \xrightarrow{1} B$

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 12.04.2016 12:20:03/Segm.S1/3	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	41.9711	Min. Time/min:	0.0
Max. Temp°C:	69.9583	Max. Time/min:	3.1325
Heating rate/(K/min):	8.934	Sampling time/s:	1.343
Sample mass/mg:	2.800		
Base line type:	tangent area prop.	LeftPts: 25	RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	68.9758	137.3423				9.1658E-2
1	E1 kJ/mol	443.3497	870.8960			+	1.3776
2	React.ord. 1	1.3483	1.8746			+	0.1189
3	log Kcat 1	0.4500	-0.1921				0.6922
4	Area 1/(J/g)	49.6585	49.6585				constant

STATISTICS

Least squares:	3.61456	Number of cycles:	20
Mean of residues:	0.16011	Max.No of cycles:	50
Correlation coefficient:	0.998061	Rel. precision:	0.001000
Durbin-Watson Value:	0.182	t-critical(0.95;74):	1.983
Durbin-Watson Factor:	2.399		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.47	74	Cn B					
1	s:	1.12	1.47	75	Fn					
2	s:	1.21	1.47	76	F2					
3	s:	1.39	1.47	75	C1 B					
4	s:	1.44	1.47	76	B1					
5	s:	4.33	1.47	75	An					
6	s:	4.61	1.47	76	A3					
7	s:	5.03	1.47	76	A2					
8	s:	6.62	1.47	76	F1					
9	s:	15.58	1.47	76	R3					
10	s:	17.56	1.47	76	D1F					
11	s:	18.46	1.47	76	D3F					
12	s:	19.50	1.47	76	D3					
13	s:	23.25	1.47	76	R2					
14	s:	32.55	1.47	76	D4					
15	s:	44.50	1.47	76	D2					
16	s:	74.08	1.47	76	D1					
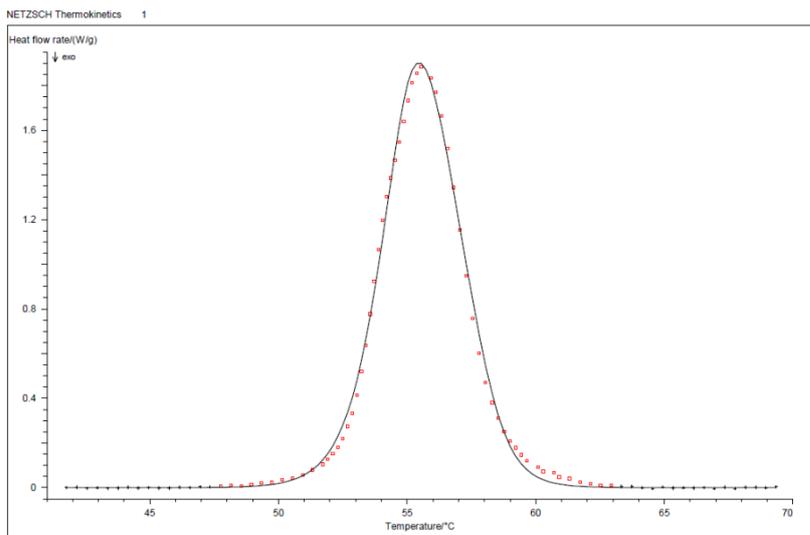
NETZSCH Thermokinetics

Date/Time: 04.10.2016 at 13:58

Project: 1
Model 1: n-th order with autocatalysis by B

$A-1\rightarrow B$

Start evaluation:	0.00050	Measurement type: DSC
Fine evaluation:	0.99950	
SCAN 1 Identity:		OP320 13.04.2016 11:49:44/Segm.S1/3
Transfer Corr:	204_F1.kcr	
Min. Temp/°C:	41.7555	Min. Time/min: 0.0
Max. Temp°C:	69.3435	Max. Time/min: 3.0976
Heating rate/(K/min):	8.906	Sampling time/s: 1.347
Sample mass/mg:	2.800	
Base line type:	tangent area prop.	LeftPts: 25 RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	62.6322	150.6634				3.7122E-2
1	E1 kJ/mol	403.1482	953.2817			+	0.7483
2	React.ord. 1	1.2389	1.8828			+	0.2630
3	log Kcat 1	0.4500	-0.5363				0.3977
4	Area 1/(J/g)	51.8524	51.8524				constant

STATISTICS

Least squares:	4.21886	Number of cycles:	22
Mean of residues:	0.17422	Max.No of cycles:	50
Correlation coefficient:	0.998023	Rel. precision:	0.001000
Durbin-Watson Value:	0.189	t-critical(0.95;73):	1.984
Durbin-Watson Factor:	2.357		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.48	73	Cn B					
1	s:	1.02	1.47	74	Fn					
2	s:	1.08	1.47	75	F2					
3	s:	1.65	1.47	74	C1 B					
4	s:	1.66	1.47	75	B1					
5	s:	4.28	1.47	74	An					
6	s:	4.38	1.47	75	A3					
7	s:	4.78	1.47	75	A2					
8	s:	6.44	1.47	75	F1					
9	s:	15.20	1.47	75	R3					
10	s:	17.76	1.47	75	D1F					
11	s:	18.55	1.47	75	D3F					
12	s:	19.41	1.47	75	D3					
13	s:	22.42	1.47	75	R2					
14	s:	31.86	1.47	75	D4					
15	s:	42.23	1.47	75	D2					
16	s:	73.18	1.47	75	D1					

Sample 18 / cycle 1 / CnB

NETZSCH Thermokinetics

Project: 1
Model 1: n-th order with autocatalysis by B

$A \longrightarrow 1 \rightarrow B$

Date/Time: 10.07.2016 at 13:11

Start evaluation:	0.00050	Measurement type: DSC
Fine evaluation:	0.99950	
SCAN 1 Identity:		OP320 27.05.2016 10:30:06/Segm.S1/3
Transfer Corr:	204_F1.kcr	
Min. Temp/°C:	41.3865	Min. Time/min: 0.0
Max. Temp°C:	56.8716	Max. Time/min: 1.7359
Heating rate/(K/min):	8.921	Sampling time/s: 1.680
Sample mass/mg:	3.360	
Base line type:		LeftPts: 20 RightPts: 10

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	257.3350	102.6031				7.4801E-2
1	E1 kJ/mol	1594.9076	645.5202			+	0.2797
2	React.ord. 1	1.2145	1.9406			+	0.1333
3	log Kcat 1	0.4500	2.1765				0.1275
4	Area 1/(J/g)	48.6894	48.6894				constant

STATISTICS

Least squares:	17.21880	Number of cycles:	19
Mean of residues:	0.52279	Max.No of cycles:	50
Correlation coefficient:	0.995851	Rel. precision:	0.001000
Durbin-Watson Value:	0.566	t-critical(0.95;24):	2.055
Durbin-Watson Factor:	1.434		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.99	24	Cn B					
1	s:	1.88	1.95	26	B1					
2	s:	2.21	1.97	25	C1 B					
3	s:	2.21	1.99	24	Bna					
4	s:	6.41	1.97	25	Fn					
5	s:	8.69	1.97	25	An					
6	s:	12.00	1.95	26	A3					
7	s:	15.28	1.95	26	F2					
8	s:	26.43	1.95	26	F1					
9	s:	32.71	1.95	26	R3					
10	s:	39.07	1.95	26	D1F					
11	s:	41.36	1.95	26	R2					
12	s:	47.31	1.95	26	D3F					
13	s:	49.03	1.95	26	D3					
14	s:	53.21	1.95	26	D4					
15	s:	56.25	1.95	26	D2					
16	s:	73.48	1.95	26	D1					
17	s:	96.93	1.95	26	A2					

Sample 18 / cycle 2 / CnB

NETZSCH Thermokinetics 1

Heat flow rate/(W/g)
↓ exo
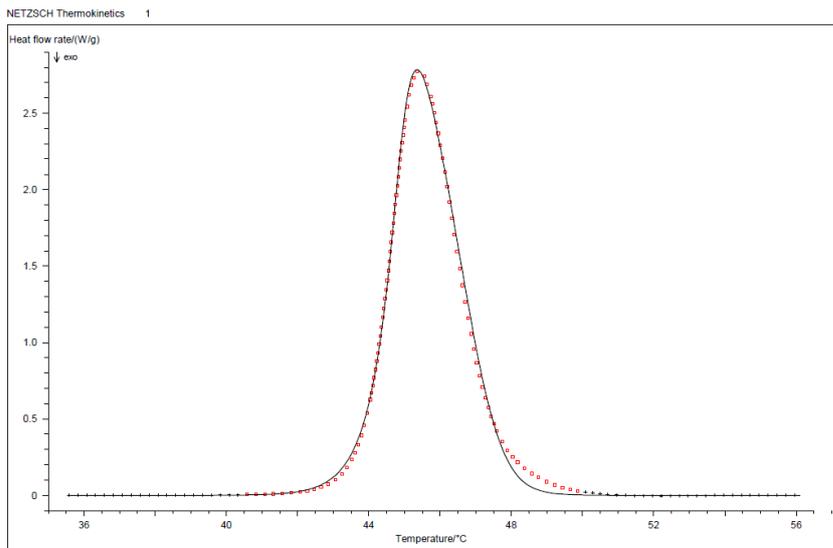
NETZSCH Thermokinetics

Date/Time: 10.07.2016 at 13:23

Project: 1
Model 1: n-th order with autocatalysis by B

A — 1→ B

Start evaluation:	0.00050	Measurement type: DSC
Fine evaluation:	0.99950	
SCAN 1 Identity:		OP320 27.05.2016 11:00:44/Segm.S1/3
Transfer Corr:	204_F1.kcr	
Min. Temp/°C:	35.5835	Min. Time/min: 0.0
Max. Temp/°C:	56.1072	Max. Time/min: 2.2997
Heating rate/(K/min):	8.925	Sampling time/s: 0.336
Sample mass/mg:	3.360	
Base line type:		LeftPts: 9 RightPts: 10

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	197.5139	216.8037				7.3589E-3
1	E1 kJ/mol	1211.0123	1328.2264			+	0.1382
2	React.ord. 1	1.7406	1.8283			+	6.8937E-2
3	log Kcat 1	0.4500	0.4443				1.6778E-2
4	Area 1/(J/g)	52.0572	52.0572				constant

STATISTICS

Least squares:	4.00618	Number of cycles:	21
Mean of residues:	9.86090E-2	Max.No of cycles:	50
Correlation coefficient:	0.999046	Rel. precision:	0.001000
Durbin-Watson Value:	0.015	t-critical(0.95;189):	1.964
Durbin-Watson Factor:	8.060		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.27	189	Cn B					
1	s:	2.85	1.27	190	C1 B					
2	s:	3.72	1.27	191	F2					
3	s:	3.74	1.27	190	Fn					
4	s:	4.19	1.27	191	B1					
5	s:	5.28	1.27	190	An					
6	s:	5.66	1.27	191	A3					
7	s:	7.60	1.27	191	A2					
8	s:	18.00	1.27	191	F1					
9	s:	37.75	1.27	191	R3					
10	s:	48.12	1.27	191	D1F					
11	s:	53.95	1.27	191	R2					
12	s:	58.23	1.27	191	D3F					
13	s:	63.93	1.27	191	D3					
14	s:	95.93	1.27	191	D4					
15	s:	122.38	1.27	191	D2					
16	s:	178.08	1.27	191	D1					
17	s:	11326.85	1.27	189	Bna					

Sample 18 / cycle 3 / CnB

NETZSCH Thermokinetics

Project: 1

Model   1: n-th order with autocatalysis by B

$A \xrightarrow{1} B$

Date/Time: 10.07.2016 at 13:39

Start evaluation:	0.00050
Fine evaluation:	0.99950
SCAN 1 Identity:	
Transfer Corr:	204_F1.kcr
Min. Temp/°C:	41.5527
Max. Temp°C:	53.7886
Heating rate/(K/min):	8.914
Sample mass/mg:	3.360
Base line type:	

Measurement type:	DSC
OP320 30.05.2016 11:22:18/Segm.S1/3	
Min. Time/min:	0.0
Max. Time/min:	1.3727
Sampling time/s:	0.336
LeftPts: 20	RightPts: 20

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	82.0888	397.8131				122.9451
1	E1 kJ/mol	509.6797	2432.2384			+	3.2639E-2
2	React.ord. 1	1.0698	2.7541			+	16.4516
3	log Kcat 1	0.4500	-4.0000				constant
4	Area 1/(J/g)	52.1588	52.1588				constant

STATISTICS

Least squares:	7.73456	Number of cycles:	11
Mean of residues:	0.17732	Max.No of cycles:	50
Correlation coefficient:	0.998718	Rel. precision:	0.001000
Durbin-Watson Value:	0.021	t-critical(0.95;148):	1.967
Durbin-Watson Factor:	6.917		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.31	148	Cn B					
1	s:	3.22	1.31	150	F2					
2	s:	4.81	1.31	149	An					
3	s:	6.53	1.31	149	C1 B					
4	s:	6.89	1.31	150	A3					
5	s:	10.35	1.31	150	A2					
6	s:	23.26	1.31	150	F1					
7	s:	42.27	1.31	150	R3					
8	s:	44.62	1.31	150	B1					
9	s:	55.86	1.31	150	D1F					
10	s:	56.54	1.31	150	R2					
11	s:	65.22	1.31	150	D3F					
12	s:	69.44	1.31	150	D3					
13	s:	96.68	1.31	150	D4					
14	s:	121.40	1.31	150	D2					
15	s:	160.19	1.31	150	D1					
16	s:	160.19	1.31	150	D1					
17	s:	160.19	1.31	150	D1					

Sample 19 / cycle 1 / CnB
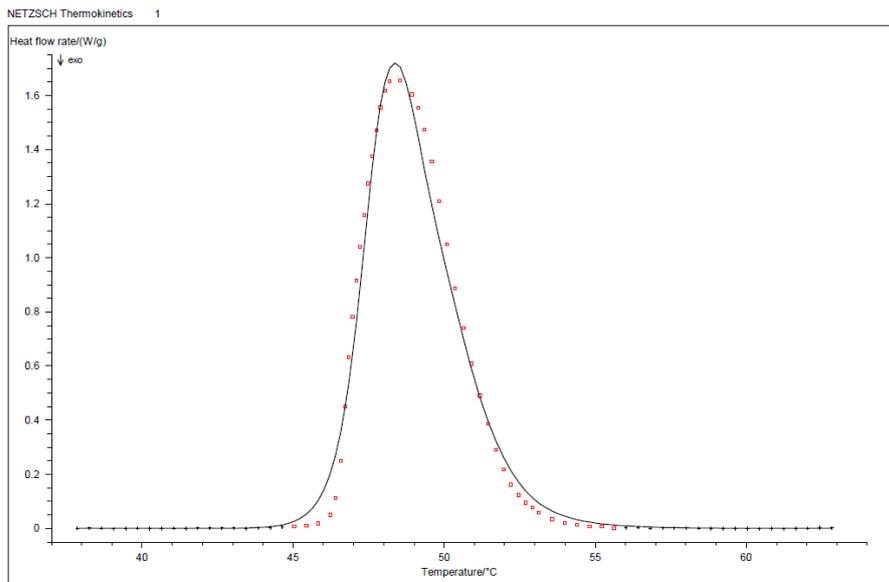
NETZSCH Thermokinetics

Date/Time: 04.10.2016 at 14:36

Project: 1
Model 1: n-th order with autocatalysis by B

$A \xrightarrow{1} B$

Start evaluation:	0.00050	Measurement type: DSC
Fine evaluation:	0.99950	
SCAN 1 Identity:		OP320 14.04.2016 13:48:15/Segm.S1/3
Transfer Corr:	204_F1.kcr	
Min. Temp/°C:	37.8548	Min. Time/min: 0.0
Max. Temp°C:	62.8357	Max. Time/min: 2.7966
Heating rate/(K/min):	8.933	Sampling time/s: 1.342
Sample mass/mg:	4.660	
Base line type:	tangent area prop.	LeftPts: 25 RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	41.5030	236.0575				0.5910
1	E1 kJ/mol	264.6496	1457.4773			+	5.2821
2	React.ord. 1	1.0837	3.3292			+	0.3867
3	log Kcat 1	0.4500	0.2742				0.9697
4	Area 1/(J/g)	43.0038	43.0038				constant

STATISTICS

Least squares:	11.70089	Number of cycles:	50
Mean of residues:	0.30474	Max.No of cycles:	50
Correlation coefficient:	0.992816	Rel. precision:	0.001000
Durbin-Watson Value:	0.164	t-critical(0.95;51):	1.998
Durbin-Watson Factor:	2.519		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.59	52	Fn					
1	s:	2.03	1.59	51	Cn B					
2	s:	3.00	1.58	53	B1					
3	s:	3.33	1.58	53	F2					
4	s:	3.52	1.59	52	C1 B					
5	s:	6.64	1.59	52	An					
6	s:	8.45	1.58	53	A2					
7	s:	12.62	1.58	53	F1					
8	s:	20.36	1.58	53	R3					
9	s:	24.62	1.58	53	D1F					
10	s:	25.64	1.58	53	R2					
11	s:	27.01	1.58	53	D3F					
12	s:	27.83	1.58	53	D3					
13	s:	36.87	1.58	53	D4					
14	s:	42.39	1.58	53	D2					
15	s:	42.70	1.59	51	Bna					
16	s:	59.45	1.58	53	D1					
17	s:	255.25	1.58	53	A3					

Sample 19 / cycle 2 / CnB

NETZSCH Thermokinetics

Date/Time: 04.10.2016 at 14:34

Project: 1
Model 1: n-th order with autocatalysis by B

$A \xrightarrow{1} B$

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 14.04.2016 15:04:45/Segm.S1/3
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	36.3948	Min. Time/min:	0.0
Max. Temp°C:	57.7620	Max. Time/min:	2.3946
Heating rate/(K/min):	8.923	Sampling time/s:	1.343
Sample mass/mg:	4.660		
Base line type:	tangent area prop.	LeftPts: 25	RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	196.3712	296.7796				0.3380
1	E1 kJ/mol	1205.5300	1816.0537			+	3.0440
2	React.ord. 1	2.3392	2.8237			+	0.3658
3	log Kcat 1	0.4500	-0.2593				1.6076
4	Area 1/(J/g)	46.6629	46.6629				constant

STATISTICS

Least squares:	6.17527	Number of cycles:	22
Mean of residues:	0.23912	Max.No of cycles:	50
Correlation coefficient:	0.997335	Rel. precision:	0.001000
Durbin-Watson Value:	0.981	t-critical(0.95;41):	2.010
Durbin-Watson Factor:	1.162		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.69	41	Cn B					
1	s:	1.02	1.68	42	Fn					
2	s:	2.29	1.67	43	F2					
3	s:	2.83	1.67	43	B1					
4	s:	2.86	1.68	42	C1 B					
5	s:	4.28	1.68	42	An					
6	s:	4.68	1.67	43	A3					
7	s:	5.94	1.67	43	A2					
8	s:	12.26	1.67	43	F1					
9	s:	21.64	1.67	43	R3					
10	s:	28.77	1.67	43	R2					
11	s:	29.66	1.67	43	D1F					
12	s:	34.65	1.67	43	D3F					
13	s:	36.13	1.67	43	D3					
14	s:	51.22	1.67	43	D4					
15	s:	57.06	1.67	43	D2					
16	s:	82.57	1.67	43	D1					
17	s:	399.97	1.69	41	Bna					

NETZSCH Thermokinetics

Date/Time: 04.10.2016 at 14:18

Project: 1
Model   1: n-th order with autocatalysis by B

A—1→B

Start evaluation:	0.00050	Measurement type: DSC
Fine evaluation:	0.99950	
SCAN 1 Identity:		OP320 14.04.2016 16:11:03/Segm.S1/3
Transfer Corr:	204_F1.kcr	
Min. Temp/°C:	34.8614	Min. Time/min: 0.0
Max. Temp°C:	59.5753	Max. Time/min: 2.7683
Heating rate/(K/min):	8.927	Sampling time/s: 1.678
Sample mass/mg:	4.660	
Base line type:	tangent area prop.	LeftPts: 25 RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	169.7908	301.4746				173.0669
1	E1 kJ/mol	1043.6406	1844.3835			+	0.3586
2	React.ord. 1	2.1842	2.7850			+	18.8609
3	log Kcat 1	0.4500	-4.0000				constant
4	Area 1/(J/g)	46.6244	46.6244				constant

STATISTICS

Least squares:	6.78102	Number of cycles:	40
Mean of residues:	0.26040	Max.No of cycles:	50
Correlation coefficient:	0.996266	Rel. precision:	0.001000
Durbin-Watson Value:	1.206	t-critical(0.95;30):	2.033
Durbin-Watson Factor:	1.089		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.83	31	Fn					
1	s:	1.01	1.58	93	A3					
2	s:	1.03	1.84	30	Cn B					
3	s:	1.82	1.82	32	F2					
4	s:	2.45	1.83	31	C1 B					
5	s:	2.51	1.82	32	B1					
6	s:	3.57	1.83	31	An					
7	s:	4.50	1.82	32	A2					
8	s:	8.99	1.82	32	F1					
9	s:	15.75	1.82	32	R3					
10	s:	20.27	1.82	32	R2					
11	s:	21.55	1.82	32	D1F					
12	s:	25.03	1.82	32	D3F					
13	s:	25.63	1.82	32	D3					
14	s:	34.34	1.82	32	D4					
15	s:	40.37	1.82	32	D2					
16	s:	61.36	1.82	32	D1					
17	s:	279.61	1.84	30	Bna					

Sample 10 / cycle 3 / Fn

NETZSCH Thermokinetics   1
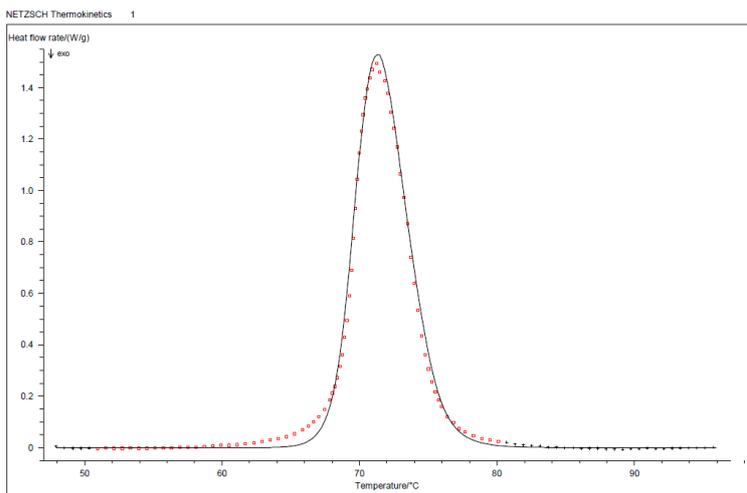
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 12:32

Project: 1
Model   1: n-th order

A—1→B

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP 320 10.11.2015 12:52:35/Segm.S1/1	
Transfer Corr:	204 F1.kcr		
Min. Temp/°C:	47.9367	Min. Time/min:	0.0
Max. Temp°C:	95.9370	Max. Time/min:	5.3622
Heating rate/(K/min):	8.952	Sampling time/s:	1.341
Sample mass/mg:	4.960		
Base line type:		LeftPts: 80	RightPts: 80

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	177.9284	176.7113				0.4344
1	E1 kJ/mol	1177.3919	1169.7892			+	2.8894
2	React.ord. 1	2.7923	2.6705			+	7.5347E-2
3	Area 1/(J/g)	51.0687	51.0687				constant

STATISTICS

Least squares:	3.20546	Number of cycles:	11
Mean of residues:	0.11533	Max.No of cycles:	50
Correlation coefficient:	0.997243	Rel. precision:	0.001000
Durbin-Watson Value:	0.090	t-critical(0.95;146):	1.967
Durbin-Watson Factor:	3.378		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.32	145	Cn B					
1	s:	1.06	1.32	147	B1					
2	s:	1.25	1.32	146	C1 B					
3	s:	1.38	1.32	146	Fn					
4	s:	2.11	1.32	147	F2					
5	s:	6.15	1.32	146	An					
6	s:	7.09	1.32	147	A2					
7	s:	10.28	1.32	147	F1					
8	s:	18.86	1.32	147	R3					
9	s:	21.59	1.32	147	D1F					
10	s:	24.29	1.32	147	D3F					
11	s:	25.29	1.32	147	D3					
12	s:	26.23	1.32	147	R2					
13	s:	38.04	1.32	147	D4					
14	s:	50.51	1.32	147	D2					
15	s:	76.55	1.32	147	D1					
16	s:	96.86	1.32	147	A3					

Sample 10 / cycle 4 / Fn
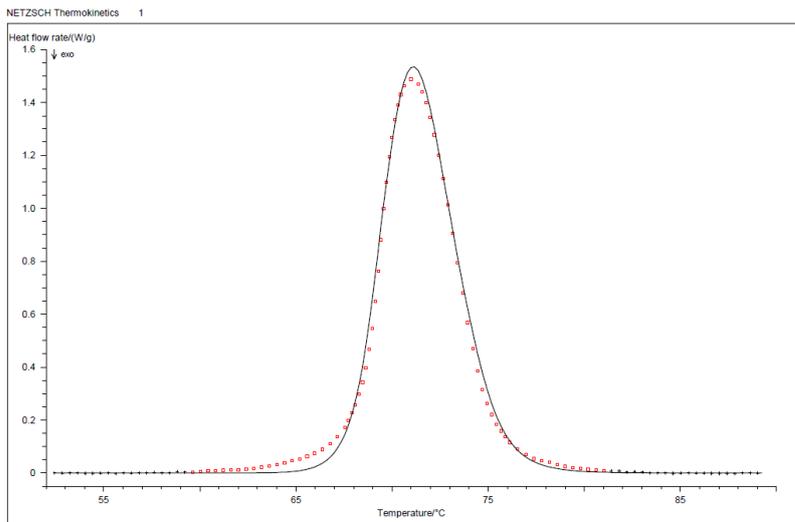
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 12:39

Project: 1
Model 1: n-th order

$A \overset{1}{\longrightarrow} B$

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP 320 10.11.2015 13:42:51/Segm.S1/1		
Transfer Corr:	204_F1.kcr			
Min. Temp/°C:	52.4361	Min. Time/min:		0.0
Max. Temp°C:	89.2324	Max. Time/min:		4.1090
Heating rate/(K/min):	8.955	Sampling time/s:		1.340
Sample mass/mg:	4.960			
Base line type:		LeftPts: 40	RightPts: 40	

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	175.2464	175.2460				3.1265E-2
1	E1 kJ/mol	1159.4749	1159.4718			+	0.2569
2	React.ord. 1	2.6002	2.6002			+	9.2144E-2
3	Area 1/(J/g)	50.7802	50.7802				constant

STATISTICS

Least squares:	3.54625	Number of cycles:	4
Mean of residues:	0.13845	Max.No of cycles:	50
Correlation coefficient:	0.997356	Rel. precision:	0.001000
Durbin-Watson Value:	0.068	t-critical(0.95;106):	1.974
Durbin-Watson Factor:	3.872		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.38	107	B1					
1	s:	1.03	1.38	105	Cn B					
2	s:	1.15	1.38	106	C1 B					
3	s:	1.31	1.38	106	Fn					
4	s:	2.00	1.38	107	F2					
5	s:	6.14	1.38	106	An					
6	s:	7.45	1.38	107	A2					
7	s:	11.00	1.38	107	F1					
8	s:	20.65	1.38	107	R3					
9	s:	23.94	1.38	107	D1F					
10	s:	26.81	1.38	107	D3F					
11	s:	27.91	1.38	107	D3					
12	s:	28.55	1.38	107	R2					
13	s:	41.03	1.38	107	D4					
14	s:	54.44	1.38	107	D2					
15	s:	80.83	1.38	107	D1					
16	s:	91.57	1.38	107	A3					
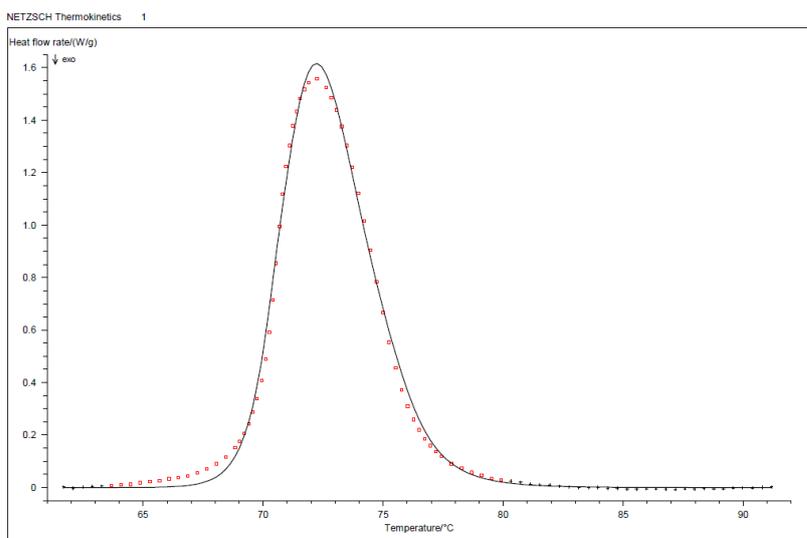
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 12:45

Project: 1
Model   1: n-th order

$$A \longrightarrow 1 \longrightarrow B$$

Start evaluation:	0.00050	Measurement type: DSC
Fine evaluation:	0.99950	
SCAN 1 Identity:		OP 320 13.11.2015 11:11:38/Segm.S1/1
Transfer Corr:	204 F1.kcr	
Min. Temp/°C:	61.6857	Min. Time/min: 0.0
Max. Temp°C:	91.1796	Max. Time/min: 3.2833
Heating rate/(K/min):	8.983	Sampling time/s: 1.340
Sample mass/mg:	4.880	
Base line type:		LeftPts: 20 RightPts: 40

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	155.6530	205.2837				2.2675E-2
1	E1 kJ/mol	1034.3960	1361.2047			+	0.2673
2	React.ord. 1	2.3412	3.0575			+	0.1436
3	Area 1/(J/g)	51.7808	51.7808				constant

STATISTICS

Least squares:	3.66961	Number of cycles:	21
Mean of residues:	0.15746	Max.No of cycles:	50
Correlation coefficient:	0.997701	Rel. precision:	0.001000
Durbin-Watson Value:	0.127	t-critical(0.95;79):	1.981
Durbin-Watson Factor:	2.854		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.45	79	Fn					
1	s:	1.01	1.46	78	Cn B					
2	s:	1.66	1.45	79	C1 B					
3	s:	1.66	1.45	80	B1					
4	s:	2.73	1.45	80	F2					
5	s:	4.76	1.45	79	An					
6	s:	9.03	1.45	80	A2					
7	s:	13.77	1.45	80	F1					
8	s:	24.37	1.45	80	R3					
9	s:	29.12	1.45	80	D1F					
10	s:	31.83	1.45	80	D3F					
11	s:	32.35	1.45	80	R2					
12	s:	32.79	1.45	80	D3					
13	s:	46.47	1.45	80	D4					
14	s:	47.59	1.45	80	A3					
15	s:	59.28	1.45	80	D2					
16	s:	87.05	1.45	80	D1					

Sample 10 / cycle 6 / Fn
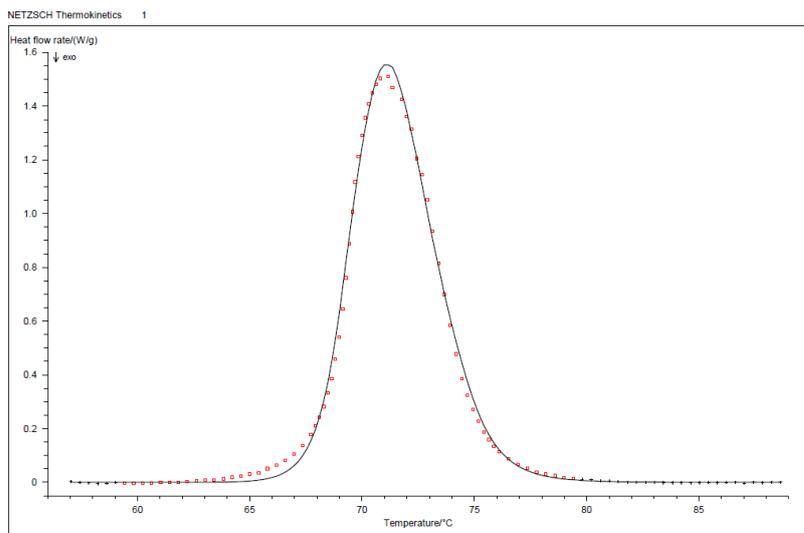
NETZSCH Thermokinetics   Date/Time: 30.11.2016 at 12:48
Project: 1
Model   1: n-th order   A—1→B

Start evaluation: 0.00050   Measurement type: DSC
Fine evaluation: 0.99950
SCAN 1   Identity: OP 320 13.11.2015 11:42:50/Segm.S1/1
Transfer Corr: 204 F1.kcr
Min. Temp/°C: 57.0308   Min. Time/min: 0.0
Max. Temp°C: 88.6342   Max. Time/min: 3.5286
Heating rate/(K/min):   8.956   Sampling time/s: 1.340
Sample mass/mg: 4.880
Base line type: LeftPts: 40   RightPts: 40

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	155.6719	184.8069				9.3586E-2
1	E1 kJ/mol	1030.9880	1222.2482			+	0.6458
2	React.ord. 1	2.3271	2.7066			+	7.0618E-2
3	Area 1/(J/g)	50.1975	50.1975				constant

STATISTICS

Least squares: 2.76174   Number of cycles: 22
Mean of residues: 0.13179   Max.No of cycles: 50
Correlation coefficient: 0.998270   Rel. precision: 0.001000
Durbin-Watson Value: 0.177   t-critical(0.95;100):   1.975
Durbin-Watson Factor: 2.429

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.39	100	Fn					
1	s:	1.01	1.40	99	Cn B					
2	s:	1.36	1.39	101	B1					
3	s:	1.46	1.39	100	C1 B					
4	s:	2.09	1.39	101	F2					
5	s:	6.73	1.39	100	An					
6	s:	9.11	1.39	101	A2					
7	s:	13.49	1.39	101	F1					
8	s:	25.28	1.39	101	R3					
9	s:	30.45	1.39	101	D1F					
10	s:	33.08	1.39	101	D3F					
11	s:	34.00	1.39	101	D3					
12	s:	34.93	1.39	101	R2					
13	s:	49.62	1.39	101	A3					
14	s:	49.66	1.39	101	D4					
15	s:	65.36	1.39	101	D2					
16	s:	98.69	1.39	101	D1					

Sample 10 / cycle 7 / Fn
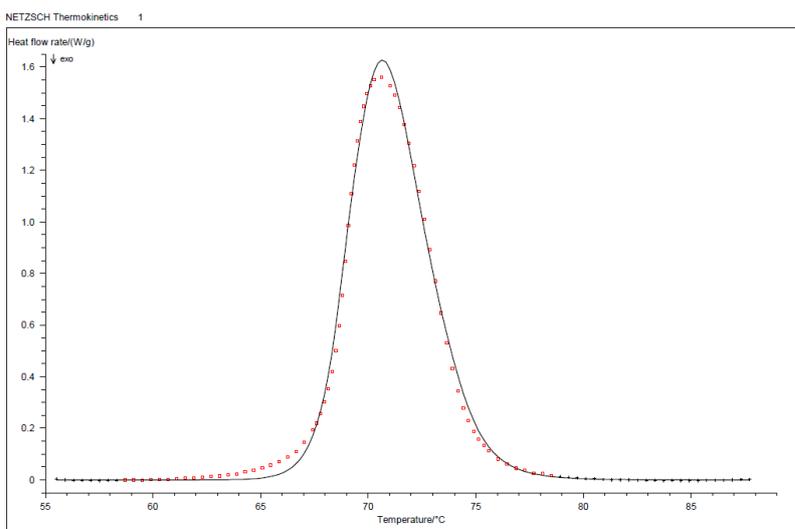
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 12:51

Project: 1
Model 1: n-th order

A—1→B

Start evaluation:	0.00050	Measurement type: DSC
Fine evaluation:	0.99950	
SCAN 1 Identity:		OP 320 16.11.2015 12:05:47/Segm.S1/1
Transfer Corr:	204 F1.kcr	
Min. Temp/°C:	55.5185	Min. Time/min: 0.0
Max. Temp°C:	87.7296	Max. Time/min: 3.5961
Heating rate/(K/min):	8.957	Sampling time/s: 1.340
Sample mass/mg:	4.830	
Base line type:		LeftPts: 40 RightPts: 40

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	151.1933	193.7903				2.1445E-2
1	E1 kJ/mol	1000.3192	1279.5762			+	0.2594
2	React.ord. 1	2.2206	2.7909			+	0.1352
3	Area 1/(J/g)	51.5447	51.5447				constant

STATISTICS

Least squares:	3.78766	Number of cycles:	23
Mean of residues:	0.15291	Max.No of cycles:	50
Correlation coefficient:	0.997733	Rel. precision:	0.001000
Durbin-Watson Value:	0.119	t-critical(0.95;98):	1.975
Durbin-Watson Factor:	2.944		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.40	98	Fn					
1	s:	1.24	1.40	99	B1					
2	s:	1.33	1.40	97	Cn B					
3	s:	1.44	1.40	98	C1 B					
4	s:	1.96	1.40	99	F2					
5	s:	5.58	1.40	98	An					
6	s:	7.16	1.40	99	A2					
7	s:	10.79	1.40	99	F1					
8	s:	19.87	1.40	99	R3					
9	s:	24.04	1.40	99	D1F					
10	s:	26.36	1.40	99	D3F					
11	s:	26.98	1.40	99	R2					
12	s:	27.19	1.40	99	D3					
13	s:	39.34	1.40	99	D4					
14	s:	51.69	1.40	99	D2					
15	s:	75.24	1.40	99	D1					
16	s:	77.18	1.40	99	A3					
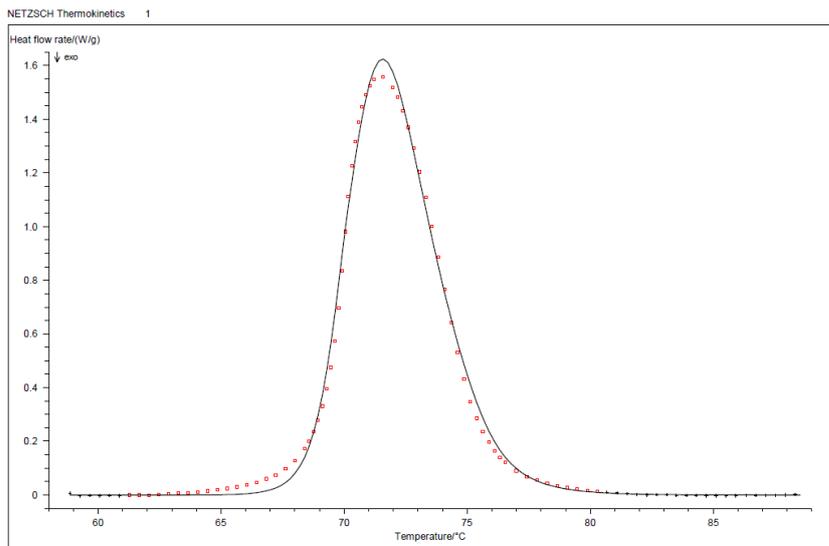
NETZSCH Thermokinetics   Date/Time: 30.11.2016 at 12:53
Project: 1
Model   1: n-th order   A—1→B

Start evaluation:		0.00050	Measurement type:		DSC
Fine evaluation:		0.99950			
SCAN 1	Identity:		OP 320 16.11.2015 10:59:19/Segm.S1/2		
Transfer Corr:		204 F1.kcr			
Min. Temp/°C:		58.8685	Min. Time/min:		0.0
Max. Temp°C:		88.5249	Max. Time/min:		3.3168
Heating rate/(K/min):		8.941	Sampling time/s:		1.345
Sample mass/mg:		4.960			
Base line type:			LeftPts: 40		RightPts: 30

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	160.3514	214.1834				2.2114E-2
1	E1 kJ/mol	1063.2886	1417.1191			+	0.2656
2	React.ord. 1	2.3791	3.1199			+	0.1441
3	Area 1/(J/g)	51.1472	51.1472				constant

STATISTICS

Least squares:	4.10163	Number of cycles:		22
Mean of residues:	0.16591	Max.No of cycles:		50
Correlation coefficient:	0.997667	Rel. precision:		0.001000
Durbin-Watson Value:	0.134	t-critical(0.95;93):		1.977
Durbin-Watson Factor:	2.774			

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.41	93	Fn					
1	s:	1.01	1.41	92	Cn B					
2	s:	1.40	1.41	94	B1					
3	s:	1.75	1.41	93	C1 B					
4	s:	2.63	1.41	94	F2					
5	s:	5.61	1.41	93	An					
6	s:	8.25	1.41	94	A2					
7	s:	12.44	1.41	94	F1					
8	s:	21.84	1.41	94	R3					
9	s:	26.41	1.41	94	D1F					
10	s:	28.93	1.41	94	D3F					
11	s:	29.12	1.41	94	R2					
12	s:	29.77	1.41	94	D3					
13	s:	42.14	1.41	94	D4					
14	s:	54.08	1.41	94	D2					
15	s:	79.96	1.41	94	D1					
16	s:	80.16	1.41	94	A3					

Sample 10 / cycle 9 / Fn

NETZSCH Thermokinetics
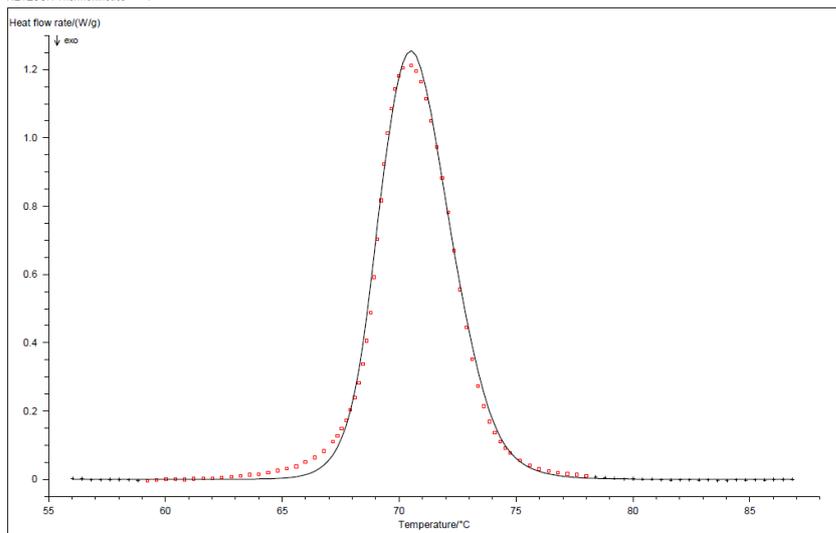
NETZSCH Thermokinetics   Date/Time: 30.11.2016 at 12:58
Project: 1
Model   1: n-th order   A —1→ B

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP 320 16.11.2015 12:37:39/Segm.S1/1
Transfer Corr:	204 F1.kcr		
Min. Temp/°C:	56.0229	Min. Time/min:	0.0
Max. Temp°C:	86.8257	Max. Time/min:	5.1556
Heating rate/(K/min):	5.975	Sampling time/s:	2.009
Sample mass/mg:	4.830		
Base line type:		LeftPts: 40	RightPts: 40

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	218.2198	211.1602				0.3882
1	E1 kJ/mol	1440.1318	1394.2123			+	2.5890
2	React.ord. 1	2.7456	2.5691			+	8.4735E-2
3	Area 1/(J/g)	50.4471	50.4471				constant

STATISTICS

Least squares:	2.05934	Number of cycles:	10
Mean of residues:	0.11527	Max.No of cycles:	50
Correlation coefficient:	0.997733	Rel. precision:	0.001000
Durbin-Watson Value:	0.118	t-critical(0.95;93):	1.977
Durbin-Watson Factor:	2.955		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.41	94	B1					
1	s:	1.11	1.41	93	C1 B					
2	s:	1.18	1.41	92	Cn B					
3	s:	1.44	1.41	93	Fn					
4	s:	2.20	1.41	94	F2					
5	s:	6.71	1.41	93	An					
6	s:	7.53	1.41	94	A3					
7	s:	8.72	1.41	94	A2					
8	s:	13.16	1.41	94	F1					
9	s:	25.17	1.41	94	R3					
10	s:	29.38	1.41	94	D1F					
11	s:	32.75	1.41	94	D3F					
12	s:	33.95	1.41	94	D3					
13	s:	35.45	1.41	94	R2					
14	s:	49.83	1.41	94	D4					
15	s:	62.41	1.41	94	D2					
16	s:	98.12	1.41	94	D1					

Sample 10 / cycle 10 / Fn

NETZSCH Thermokinetics   Date/Time: 30.11.2016 at 13:12
Project: 1
Model   1: n-th order   A—1→B

Start evaluation: 0.00050   Measurement type: DSC
Fine evaluation: 0.99950
SCAN 1   Identity: OP 320 16.11.2015 13:22:15/Segm.S1/1
Transfer Corr: 204_F1.kcr
Min. Temp/°C: 55.3712   Min. Time/min: 0.0
Max. Temp°C: 91.3669   Max. Time/min: 3.0129
Heating rate/(K/min):   11.947   Sampling time/s: 1.004
Sample mass/mg: 4.830
Base line type: LeftPts: 40   RightPts: 40

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	127.9042	172.2243				0.1140
1	E1 kJ/mol	847.2056	1137.6793			+	0.7803
2	React.ord. 1	2.1922	2.8824			+	7.8872E-2
3	Area 1/(J/g)	52.1064	52.1064				constant

STATISTICS

Least squares:	5.86180	Number of cycles:	21
Mean of residues:	0.17996	Max.No of cycles:	50
Correlation coefficient:	0.997525	Rel. precision:	0.001000
Durbin-Watson Value:	0.099	t-critical(0.95;117):	1.971
Durbin-Watson Factor:	3.221		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.36	117	Fn					
1	s:	1.32	1.36	116	Cn B					
2	s:	1.44	1.36	117	C1 B					
3	s:	2.04	1.36	118	F2					
4	s:	5.22	1.36	117	An					
5	s:	5.23	1.36	118	B1					
6	s:	6.98	1.36	118	A2					
7	s:	10.33	1.36	118	F1					
8	s:	18.68	1.36	118	R3					
9	s:	22.51	1.36	118	D1F					
10	s:	24.61	1.36	118	D3F					
11	s:	25.12	1.36	118	R2					
12	s:	25.31	1.36	118	D3					
13	s:	36.47	1.36	118	D4					
14	s:	48.03	1.36	118	D2					
15	s:	64.38	1.36	118	A3					
16	s:	70.47	1.36	118	D1					

Sample 11 / cycle 1 / Fn

NETZSCH Thermokinetics 1
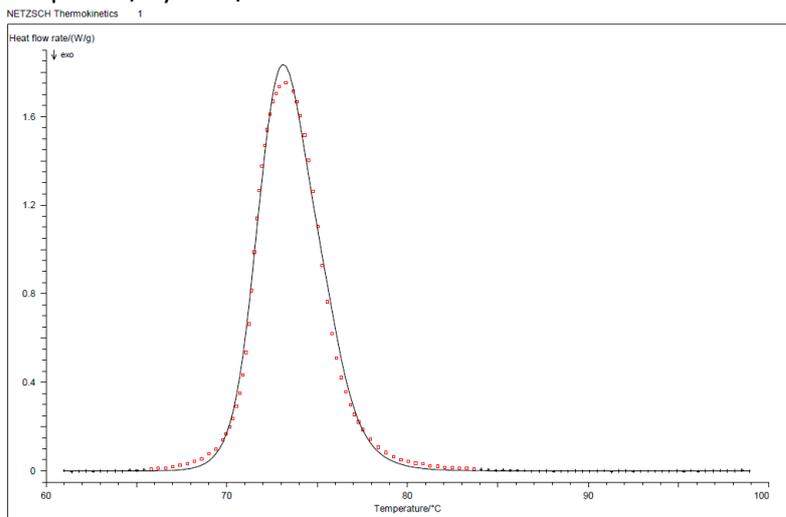
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 13:48

Project: 1
Model   1: n-th order

A—1→B

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP320 21.04.2016 17:11:05/Segm.S2/3		
Transfer Corr:	204 F1.kcr			
Min. Temp/°C:	61.0056	Min. Time/min:		0.0
Max. Temp°C:	98.8907	Max. Time/min:		4.2167
Heating rate/(K/min):	8.984	Sampling time/s:		1.339
Sample mass/mg:	3.870			
Base line type:		LeftPts: 25		RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	148.9849	200.9381				2.2954E-2
1	E1 kJ/mol	993.3331	1336.3436			+	0.3001
2	React.ord. 1	2.0858	2.7147			+	0.1550
3	Area 1/(J/g)	54.5068	54.5068				constant

STATISTICS

Least squares:	3.90971	Number of cycles:	23
Mean of residues:	0.14345	Max.No of cycles:	50
Correlation coefficient:	0.997630	Rel. precision:	0.001000
Durbin-Watson Value:	0.171	t-critical(0.95;88):	1.978
Durbin-Watson Factor:	2.473		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.43	88	Fn					
1	s:	1.28	1.43	87	Cn B					
2	s:	1.55	1.42	89	B1					
3	s:	1.59	1.43	88	C1 B					
4	s:	1.83	1.42	89	F2					
5	s:	5.46	1.43	88	An					
6	s:	7.32	1.42	89	A2					
7	s:	10.31	1.42	89	F1					
8	s:	16.62	1.42	89	A3					
9	s:	18.86	1.42	89	R3					
10	s:	22.46	1.42	89	D1F					
11	s:	24.05	1.42	89	D3F					
12	s:	24.76	1.42	89	D3					
13	s:	25.25	1.42	89	R2					
14	s:	35.83	1.42	89	D4					
15	s:	44.65	1.42	89	D2					
16	s:	69.13	1.42	89	D1					

Sample 11 / cycle 2 / Fn
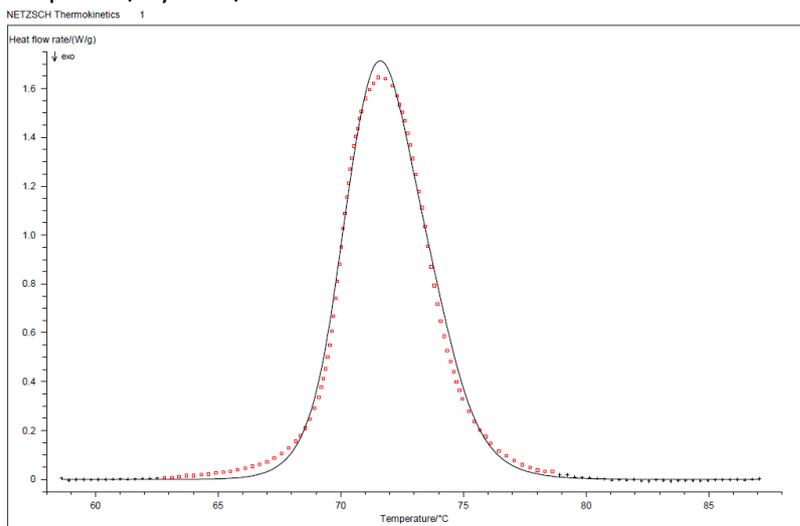
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 13:58

Project: 1
Model   1: n-th order

$A \xrightarrow{1} B$

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 22.04.2016 12:59:05/Segm.S1/2	
Transfer Corr:	204 F1.kcr		
Min. Temp/°C:	58.6101	Min. Time/min:	0.0
Max. Temp°C:	87.0675	Max. Time/min:	3.1823
Heating rate/(K/min):	8.943	Sampling time/s:	0.672
Sample mass/mg:	3.870		
Base line type:		LeftPts: 80	RightPts: 60

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	138.1023	183.2205				7.9662E-2
1	E1 kJ/mol	917.4334	1213.9596			+	0.5554
2	React.ord. 1	1.8396	2.4320			+	6.1316E-2
3	Area 1/(J/g)	51.2669	51.2669				constant

STATISTICS

Least squares:	4.28818	Number of cycles:	18
Mean of residues:	0.12266	Max.No of cycles:	50
Correlation coefficient:	0.997585	Rel. precision:	0.001000
Durbin-Watson Value:	0.044	t-critical(0.95;159):	1.966
Durbin-Watson Factor:	4.800		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.30	159	Fn					
1	s:	1.21	1.30	160	B1					
2	s:	1.28	1.30	159	C1 B					
3	s:	1.38	1.30	160	F2					
4	s:	1.48	1.30	158	Cn B					
5	s:	5.07	1.30	159	An					
6	s:	5.76	1.30	160	A3					
7	s:	6.53	1.30	160	A2					
8	s:	9.16	1.30	160	F1					
9	s:	17.75	1.30	160	R3					
10	s:	20.83	1.30	160	D1F					
11	s:	22.45	1.30	160	D3F					
12	s:	23.23	1.30	160	D3					
13	s:	24.64	1.30	160	R2					
14	s:	35.59	1.30	160	D4					
15	s:	46.30	1.30	160	D2					
16	s:	71.50	1.30	160	D1					

Sample 11 / cycle 3 / Fn

NETZSCH Thermokinetics   1
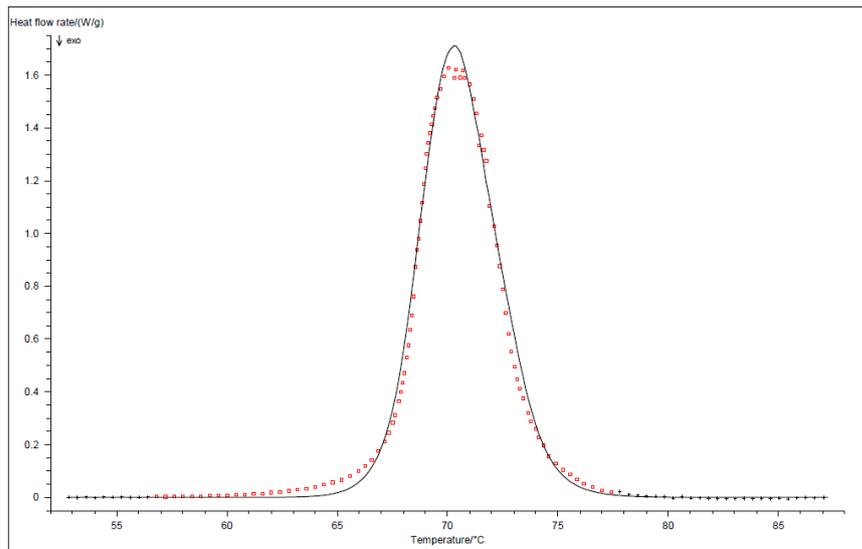
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 14:01

Project: 1
Model   1: n-th order   A —1→ B

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 22.04.2016 13:30:23/Segm.S1/2	
Transfer Corr:	204 F1.kcr		
Min. Temp/°C:	52.8214	Min. Time/min:	0.0
Max. Temp°C:	87.2370	Max. Time/min:	3.8442
Heating rate/(K/min):	8.953	Sampling time/s:	0.671
Sample mass/mg:	3.870		
Base line type:		LeftPts: 80	RightPts: 80

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	128.1791	173.4898				8.7350E-2
1	E1 kJ/mol	848.8379	1145.4713			+	0.6070
2	React.ord. 1	1.7230	2.3204			+	6.4286E-2
3	Area 1/(J/g)	51.6411	51.6411				constant

STATISTICS

Least squares:	5.11376	Number of cycles:	14
Mean of residues:	0.12175	Max.No of cycles:	50
Correlation coefficient:	0.996928	Rel. precision:	0.001000
Durbin-Watson Value:	0.158	t-critical(0.95;204):	1.963
Durbin-Watson Factor:	2.569		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.26	204	Fn					
1	s:	1.02	1.26	205	B1					
2	s:	1.04	1.26	204	C1 B					
3	s:	1.15	1.26	205	F2					
4	s:	1.19	1.26	203	Cn B					
5	s:	3.86	1.26	204	An					
6	s:	3.97	1.26	205	A3					
7	s:	4.35	1.26	205	A2					
8	s:	6.00	1.26	205	F1					
9	s:	11.60	1.26	205	R3					
10	s:	13.64	1.26	205	D1F					
11	s:	14.72	1.26	205	D3F					
12	s:	15.21	1.26	205	D3					
13	s:	16.19	1.26	205	R2					
14	s:	23.66	1.26	205	D4					
15	s:	31.39	1.26	205	D2					
16	s:	49.08	1.26	205	D1					

Sample 11 / cycle 4 / Fn
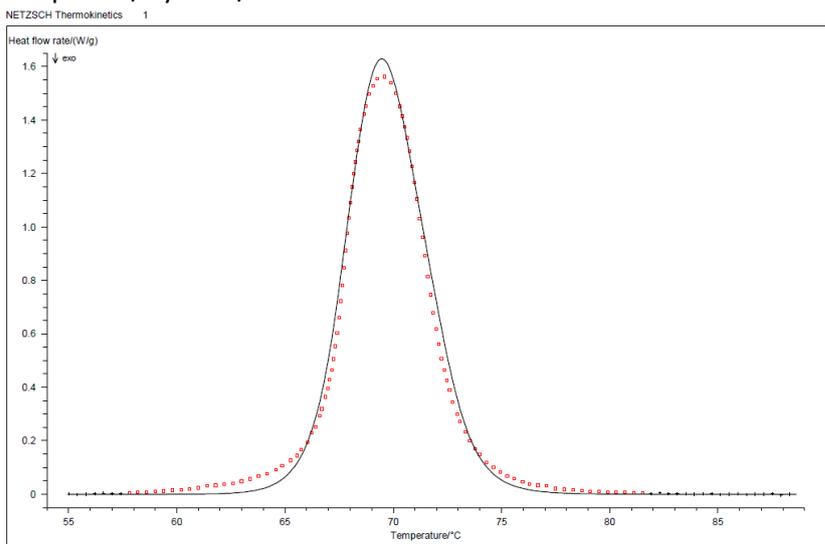
NETZSCH Thermokinetics

Project: 1

Model 1: n-th order

Date/Time: 30.11.2016 at 14:06

A—1→B

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 22.04.2016 14:15:05/Segm.S1/2	
Transfer Corr:	204 F1.kcr		
Min. Temp/°C:	55.0104	Min. Time/min:	0.0
Max. Temp°C:	88.6123	Max. Time/min:	3.7561
Heating rate/(K/min):	8.946	Sampling time/s:	0.671
Sample mass/mg:	3.870		
Base line type:		LeftPts: 40	RightPts: 40

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	143.7636	159.3734				0.2045
1	E1 kJ/mol	948.5039	1050.4797			+	1.3778
2	React.ord. 1	2.0385	2.2334			+	6.5431E-2
3	Area 1/(J/g)	51.6792	51.6792				constant

STATISTICS

Least squares:	5.55452	Number of cycles:	7
Mean of residues:	0.12838	Max.No of cycles:	50
Correlation coefficient:	0.996625	Rel. precision:	0.001000
Durbin-Watson Value:	0.024	t-critical(0.95;237):	1.961
Durbin-Watson Factor:	6.487		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.24	237	C1 B					
1	s:	1.01	1.24	238	B1					
2	s:	1.05	1.24	236	Cn B					
3	s:	1.44	1.24	237	Fn					
4	s:	1.54	1.24	238	F2					
5	s:	4.03	1.24	237	An					
6	s:	4.71	1.24	238	A3					
7	s:	5.31	1.24	238	A2					
8	s:	7.28	1.24	238	F1					
9	s:	14.27	1.24	238	R3					
10	s:	15.78	1.24	238	D1F					
11	s:	17.52	1.24	238	D3F					
12	s:	18.40	1.24	238	D3					
13	s:	20.03	1.24	238	R2					
14	s:	29.21	1.24	238	D4					
15	s:	37.71	1.24	238	D2					
16	s:	58.72	1.24	238	D1					

Sample 11 / cycle 5 / Fn

NETZSCH Thermokinetics   1
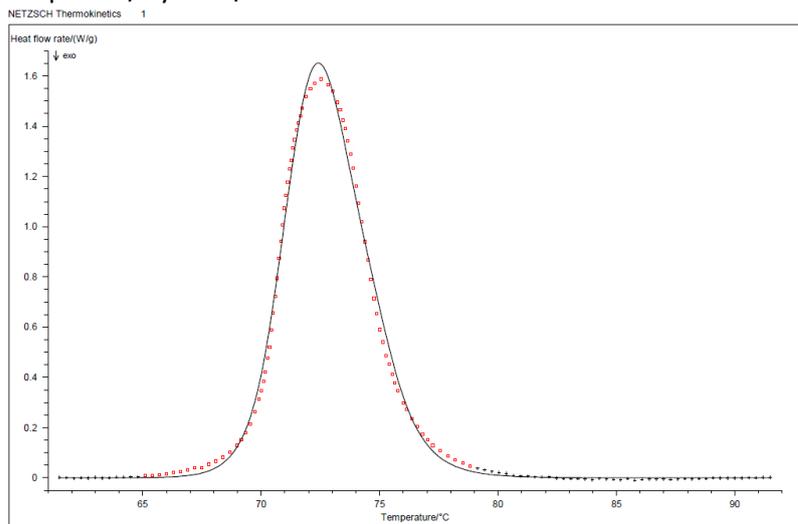
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 14:13

Project: 1
Model   1: n-th order

A—1→B

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 26.04.2016 11:13:10/Segm.S1/2	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	61.4923	Min. Time/min:	0.0
Max. Temp°C:	91.4874	Max. Time/min:	3.3423
Heating rate/(K/min):	8.974	Sampling time/s:	0.671
Sample mass/mg:	3.870		
Base line type:		LeftPts: 30	RightPts: 80

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	187.3333	187.3333				1.7556E-2
1	E1 kJ/mol	1243.9742	1243.9742			+	0.2293
2	React.ord. 1	2.5402	2.5402			+	0.1159
3	Area 1/(J/g)	49.1985	49.1985				constant

STATISTICS

Least squares:	3.51731	Number of cycles:	14
Mean of residues:	0.10828	Max.No of cycles:	50
Correlation coefficient:	0.997558	Rel. precision:	0.001000
Durbin-Watson Value:	0.058	t-critical(0.95;137):	1.968
Durbin-Watson Factor:	4.180		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.33	136	Bna					
1	s:	1.01	1.33	137	Fn					
2	s:	1.01	1.33	136	Cn B					
3	s:	1.64	1.33	138	F2					
4	s:	1.65	1.33	138	B1					
5	s:	1.84	1.33	137	C1 B					
6	s:	5.61	1.33	137	An					
7	s:	6.96	1.33	138	A3					
8	s:	8.06	1.33	138	A2					
9	s:	11.08	1.33	138	F1					
10	s:	20.95	1.33	138	R3					
11	s:	24.77	1.33	138	D1F					
12	s:	26.06	1.33	138	D3F					
13	s:	26.76	1.33	138	D3					
14	s:	28.67	1.33	138	R2					
15	s:	40.24	1.33	138	D4					
16	s:	53.45	1.33	138	D2					
17	s:	80.13	1.33	138	D1					

Sample 11 / cycle 6 / Fn

NETZSCH Thermokinetics   1
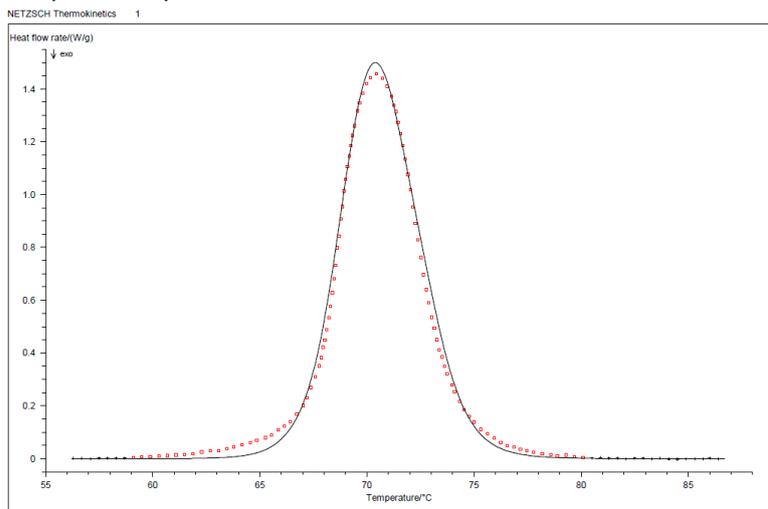
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 14:17

Project: 1
Model   1: n-th order

$A \xrightarrow{1} B$

Start evaluation:	0.00050	Measurement type: DSC
Fine evaluation:	0.99950	
SCAN 1 Identity:		OP320 26.04.2016 13:08:26/Segm.S1/2
Transfer Corr:	204 F1.kcr	
Min. Temp/°C:	55.9890	Min. Time/min: 0.0
Max. Temp/°C:	86.4000	Max. Time/min: 3.3963
Heating rate/(K/min):	8.954	Sampling time/s: 0.670
Sample mass/mg:	3.870	
Base line type:		LeftPts: 70 RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	141.7254	153.5169				0.1854
1	E1 kJ/mol	937.6999	1014.9295			+	1.2548
2	React.ord. 1	2.0389	2.2035			+	6.2383E-2
3	Area 1/(J/g)	48.3202	48.3202				constant

STATISTICS

Least squares:	4.34836	Number of cycles:	6
Mean of residues:	0.11940	Max.No of cycles:	50
Correlation coefficient:	0.997120	Rel. precision:	0.001000
Durbin-Watson Value:	0.028	t-critical(0.95;217):	1.962
Durbin-Watson Factor:	5.945		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.25	217	C1 B					
1	s:	1.01	1.25	218	B1					
2	s:	1.04	1.25	216	Cn B					
3	s:	1.56	1.25	217	Fn					
4	s:	1.67	1.25	218	F2					
5	s:	1.98	1.30	136	Bna					
6	s:	5.34	1.25	217	An					
7	s:	6.29	1.25	218	A3					
8	s:	7.05	1.25	218	A2					
9	s:	9.44	1.25	218	F1					
10	s:	18.95	1.25	218	R3					
11	s:	20.54	1.25	218	D1F					
12	s:	22.67	1.25	218	D3F					
13	s:	23.83	1.25	218	D3					
14	s:	26.76	1.25	218	R2					
15	s:	37.49	1.25	218	D4					
16	s:	49.12	1.25	218	D2					
17	s:	78.10	1.25	218	D1					

Sample 11 / cycle 7 / Fn

NETZSCH Thermokinetics   1
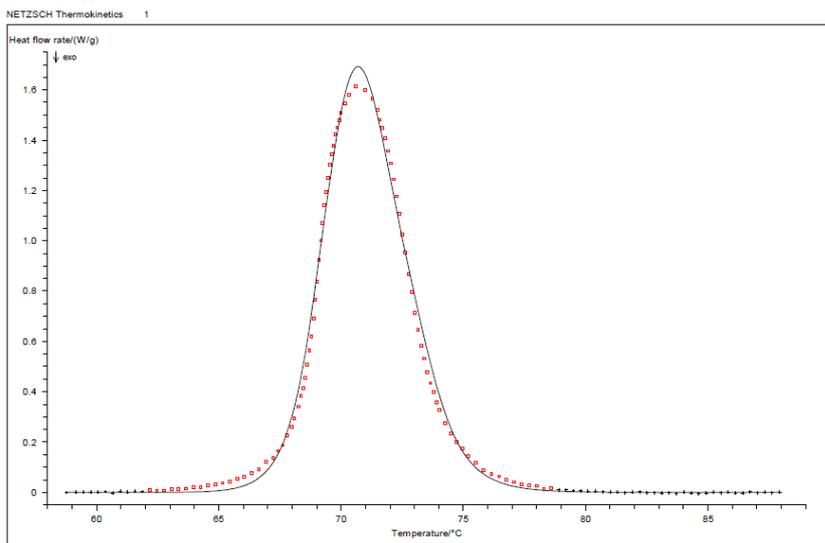
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 14:19

Project: 1
Model   1: n-th order

A—1→B

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950
SCAN 1 Identity:		OP320 26.04.2016 13:49:33/Segm.S2/3
Transfer Corr:	204 F1.kcr
Min. Temp/°C:	58.7664	Min. Time/min:	0.0
Max. Temp°C:	88.0168	Max. Time/min:	3.2574
Heating rate/(K/min):	8.980	Sampling time/s:	0.669
Sample mass/mg:	3.770
Base line type:		LeftPts: 25	RightPts: 45

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	186.5360	186.5360				1.7208E-2
1	E1 kJ/mol	1232.4762	1232.4762			+	0.2275
2	React.ord. 1	2.4867	2.4867			+	0.1146
3	Area 1/(J/g)	49.7442	49.7442				constant

STATISTICS

Least squares:	4.31777	Number of cycles:	14
Mean of residues:	0.12139	Max.No of cycles:	50
Correlation coefficient:	0.997483	Rel. precision:	0.001000
Durbin-Watson Value:	0.058	t-critical(0.95;163):	1.966
Durbin-Watson Factor:	4.196		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.30	162	Bna					
1	s:	1.11	1.30	163	Fn					
2	s:	1.12	1.30	162	Cn B					
3	s:	1.53	1.30	164	B1					
4	s:	1.60	1.30	164	F2					
5	s:	1.63	1.30	163	C1 B					
6	s:	5.54	1.30	163	An					
7	s:	6.34	1.30	164	A3					
8	s:	7.22	1.30	164	A2					
9	s:	9.99	1.30	164	F1					
10	s:	19.10	1.30	164	R3					
11	s:	22.70	1.30	164	D1F					
12	s:	24.07	1.30	164	D3F					
13	s:	24.74	1.30	164	D3					
14	s:	26.36	1.30	164	R2					
15	s:	37.47	1.30	164	D4					
16	s:	50.09	1.30	164	D2					
17	s:	76.35	1.30	164	D1					

Sample 11 / cycle 8 / Fn

NETZSCH Thermokinetics   1
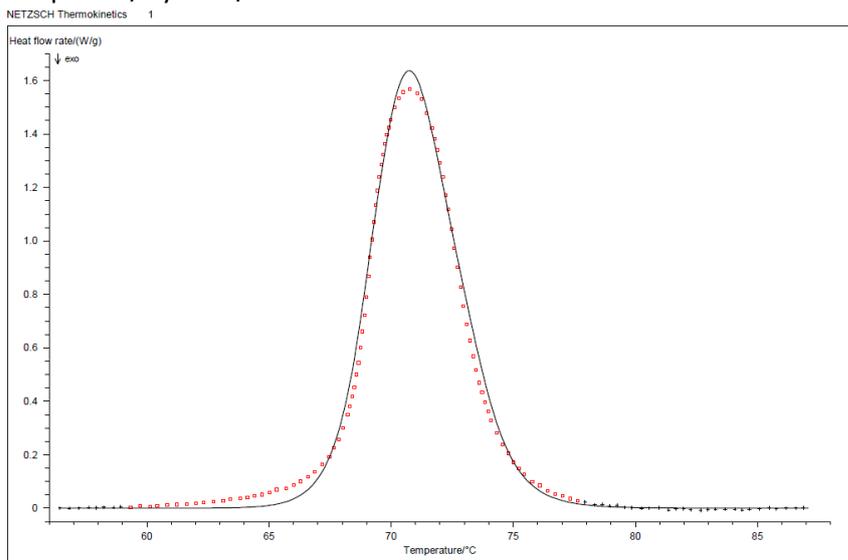
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 14:23

Project: 1
Model   1: n-th order

$A {-\!1\!\rightarrow} B$

Start evaluation:	0.00050	Measurement type: DSC
Fine evaluation:	0.99950	
SCAN 1 Identity:		OP320 27.04.2016 15:05:36/Segm.S1/2
Transfer Corr:	204 F1.kcr	
Min. Temp/°C:	56.4318	Min. Time/min: 0.0
Max. Temp°C:	87.0779	Max. Time/min: 3.4272
Heating rate/(K/min):	8.942	Sampling time/s: 0.672
Sample mass/mg:	3.770	
Base line type:		LeftPts: 20 RightPts: 70

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	172.7381	172.7201				4.5784E-2
1	E1 kJ/mol	1142.0803	1141.9622			+	0.3375
2	React.ord. 1	2.3893	2.3890			+	6.8513E-2
3	Area 1/(J/g)	50.3020	50.3020				constant

STATISTICS

Least squares:	5.05118	Number of cycles:	2
Mean of residues:	0.12827	Max.No of cycles:	50
Correlation coefficient:	0.996880	Rel. precision:	0.001000
Durbin-Watson Value:	0.031	t-critical(0.95;184):	1.964
Durbin-Watson Factor:	5.709		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.28	185	B1					
1	s:	1.02	1.29	162	Bna					
2	s:	1.03	1.28	184	C1 B					
3	s:	1.07	1.28	183	Cn B					
4	s:	1.17	1.28	184	Fn					
5	s:	1.43	1.28	185	F2					
6	s:	4.58	1.28	184	An					
7	s:	5.14	1.28	185	A3					
8	s:	5.75	1.28	185	A2					
9	s:	7.83	1.28	185	F1					
10	s:	15.04	1.28	185	R3					
11	s:	17.03	1.28	185	D1F					
12	s:	18.59	1.28	185	D3F					
13	s:	19.33	1.28	185	D3					
14	s:	21.03	1.28	185	R2					
15	s:	29.52	1.28	185	D4					
16	s:	39.11	1.28	185	D2					
17	s:	60.72	1.28	185	D1					

Sample 11 / cycle 9 / Fn
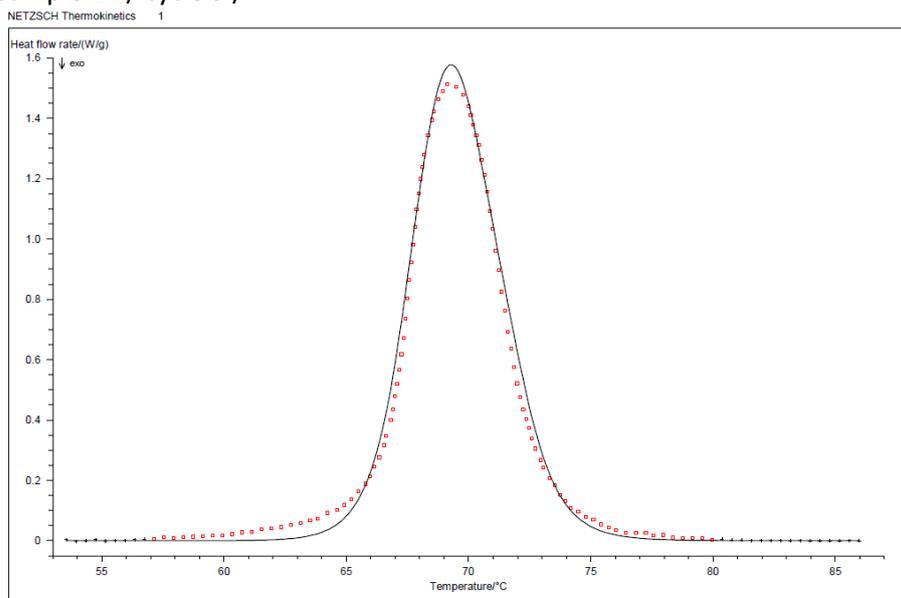
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 14:27

Project: 1
Model   1: n-th order

$A \xrightarrow{1} B$

Start evaluation:	0.00050	Measurement type:			DSC
Fine evaluation:	0.99950				
SCAN 1 Identity:		OP320 27.04.2016 15:44:57/Segm.S1/2			
Transfer Corr:	204 F1.kcr				
Min. Temp/°C:	53.5533	Min. Time/min:			0.0
Max. Temp°C:	85.9643	Max. Time/min:			3.6271
Heating rate/(K/min):	8.936	Sampling time/s:			0.672
Sample mass/mg:	3.770				
Base line type:		LeftPts: 80		RightPts: 20	

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum Sign	t*Std.Dev.
0	log A1/s^-1	135.1801	156.4270			0.2126
1	E1 kJ/mol	891.9617	1030.6636		+	1.4311
2	React.ord. 1	1.9448	2.2406		+	6.7675E-2
3	Area 1/(J/g)	50.4746	50.4746			constant

STATISTICS

Least squares:	5.56186	Number of cycles:	6
Mean of residues:	0.13082	Max.No of cycles:	50
Correlation coefficient:	0.996465	Rel. precision:	0.001000
Durbin-Watson Value:	0.027	t-critical(0.95;227):	1.962
Durbin-Watson Factor:	6.105		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.25	228	B1					
1	s:	1.01	1.25	227	C1 B					
2	s:	1.08	1.25	226	Cn B					
3	s:	1.40	1.28	162	Bna					
4	s:	1.44	1.25	227	Fn					
5	s:	1.55	1.25	228	F2					
6	s:	4.43	1.25	227	An					
7	s:	4.90	1.25	228	A3					
8	s:	5.42	1.25	228	A2					
9	s:	7.25	1.25	228	F1					
10	s:	14.15	1.25	228	R3					
11	s:	15.48	1.25	228	D1F					
12	s:	17.14	1.25	228	D3F					
13	s:	17.96	1.25	228	D3					
14	s:	19.80	1.25	228	R2					
15	s:	28.14	1.25	228	D4					
16	s:	36.89	1.25	228	D2					
17	s:	57.73	1.25	228	D1					

Sample 11 / cycle 10 / Fn

NETZSCH Thermokinetics
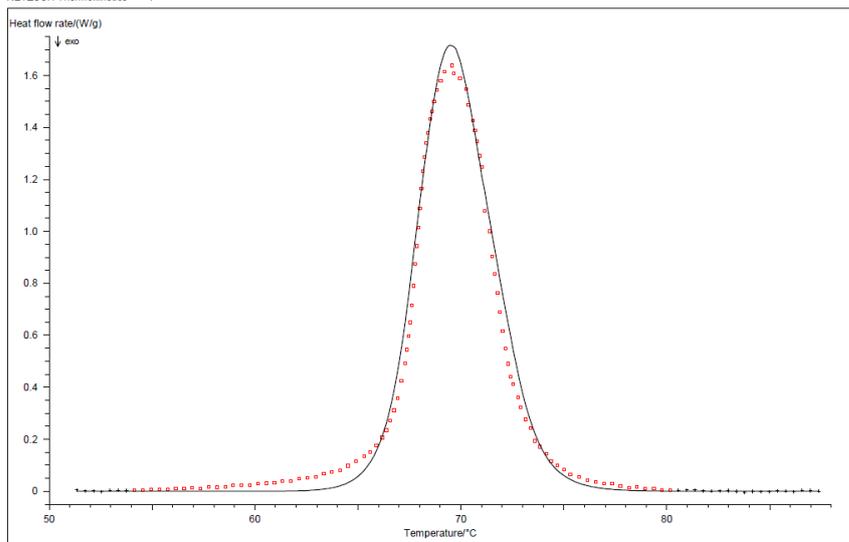
Date/Time: 30.11.2016 at 14:43

Project: 1
Model   1: n-th order

$$A \xrightarrow{1} B$$

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 27.04.2016 17:04:37/Segm.S2/3	
Transfer Corr:	204 F1.kcr		
Min. Temp/°C:	51.3537	Min. Time/min:	0.0
Max. Temp°C:	87.3781	Max. Time/min:	4.0164
Heating rate/(K/min):	8.969	Sampling time/s:	0.669
Sample mass/mg:	3.770		
Base line type:		LeftPts: 120	RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	165.4667	165.4662				2.9871E-2
1	E1 kJ/mol	1090.3762	1090.3729			+	0.2511
2	React.ord. 1	2.3234	2.3233			+	8.7277E-2
3	Area 1/(J/g)	53.8953	53.8953				constant

STATISTICS

Least squares:	9.58381	Number of cycles:	4
Mean of residues:	0.16294	Max.No of cycles:	50
Correlation coefficient:	0.994427	Rel. precision:	0.001000
Durbin-Watson Value:	0.063	t-critical(0.95;262):	1.960
Durbin-Watson Factor:	4.022		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.23	261	Cn B					
1	s:	1.08	1.23	263	B1					
2	s:	1.09	1.23	262	C1 B					
3	s:	1.58	1.23	262	Fn					
4	s:	1.69	1.23	263	F2					
5	s:	3.46	1.23	262	An					
6	s:	4.01	1.23	263	A2					
7	s:	5.38	1.23	263	F1					
8	s:	6.01	1.23	263	A3					
9	s:	9.68	1.23	263	R3					
10	s:	10.63	1.23	263	D1F					
11	s:	11.95	1.23	263	D3F					
12	s:	12.53	1.23	263	D3					
13	s:	13.22	1.23	263	R2					
14	s:	19.13	1.23	263	D4					
15	s:	25.87	1.23	263	D2					
16	s:	38.28	1.23	263	D1					
17	s:	2452.59	1.23	261	Bna					

Sample 11 / cycle 11 / Fn

NETZSCH Thermokinetics   1
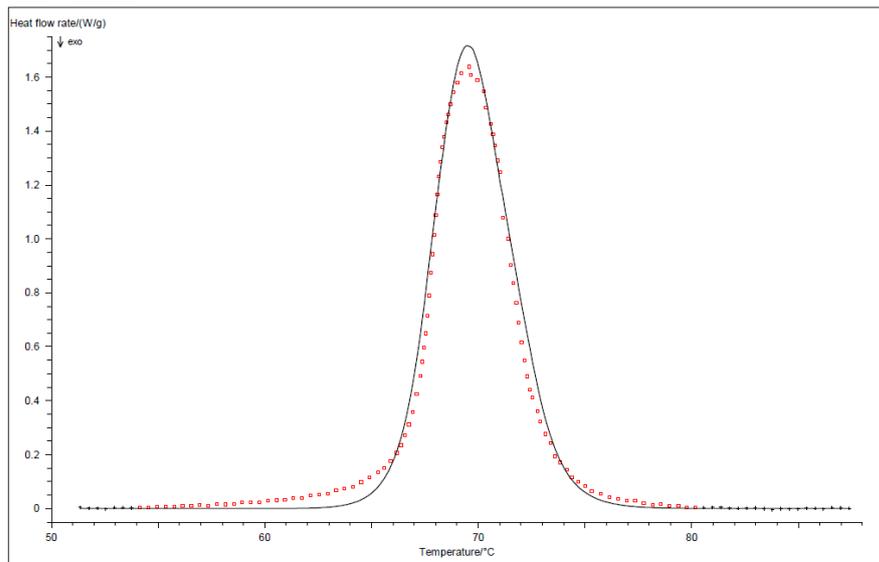
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 14:45

Project: 1
Model   1: n-th order

A—1→B

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP320 27.04.2016 17:04:37/Segm.S2/3		
Transfer Corr:	204 F1.kcr			
Min. Temp/°C:	51.3537	Min. Time/min:		0.0
Max. Temp/°C:	87.3781	Max. Time/min:		4.0164
Heating rate/(K/min):	8.969	Sampling time/s:		0.669
Sample mass/mg:	3.770			
Base line type:		LeftPts: 120		RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	133.0351	165.4667				0.5872
1	E1 kJ/mol	878.5152	1090.3762			+	3.8806
2	React.ord. 1	1.8725	2.3234			+	7.5052E-2
3	Area 1/(J/g)	53.8953	53.8953				constant

STATISTICS

Least squares:	9.58381	Number of cycles:	11
Mean of residues:	0.16294	Max.No of cycles:	50
Correlation coefficient:	0.994427	Rel. precision:	0.001000
Durbin-Watson Value:	0.063	t-critical(0.95;262):	1.960
Durbin-Watson Factor:	4.022		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.23	261	Cn B					
1	s:	1.08	1.23	263	B1					
2	s:	1.09	1.23	262	C1 B					
3	s:	1.58	1.23	262	Fn					
4	s:	1.69	1.23	263	F2					
5	s:	3.46	1.23	262	An					
6	s:	4.01	1.23	263	A2					
7	s:	5.38	1.23	263	F1					
8	s:	6.01	1.23	263	A3					
9	s:	9.68	1.23	263	R3					
10	s:	10.63	1.23	263	D1F					
11	s:	11.95	1.23	263	D3F					
12	s:	12.53	1.23	263	D3					
13	s:	13.22	1.23	263	R2					
14	s:	19.13	1.23	263	D4					
15	s:	25.87	1.23	263	D2					
16	s:	38.28	1.23	263	D1					
17	s:	2452.59	1.23	261	Bna					

Sample 11 / cycle 12 / Fn

NETZSCH Thermokinetics   1

Heat flow rate/(W/g)

Temperature/°C

NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 14:48

Project: 1
Model   1: n-th order

A—1→B

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP320 28.04.2016 12:45:11/Segm.S2/3		
Transfer Corr:	204 F1.kcr			
Min. Temp/°C:	61.3647	Min. Time/min:		0.0
Max. Temp°C:	92.4703	Max. Time/min:		3.4614
Heating rate/(K/min):	8.986	Sampling time/s:		0.670
Sample mass/mg:	3.770			
Base line type:		LeftPts: 10	RightPts: 50	

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum Sign	t*Std.Dev.
0	log A1/s^-1	125.7539	192.0209			1.9415E-2
1	E1 kJ/mol	833.8036	1268.1077		+	0.2644
2	React.ord. 1	1.6629	2.5028		+	0.1340
3	Area 1/(J/g)	48.8046	48.8046			constant

STATISTICS

Least squares:	4.04275	Number of cycles:	21
Mean of residues:	0.11401	Max.No of cycles:	50
Correlation coefficient:	0.997146	Rel. precision:	0.001000
Durbin-Watson Value:	0.060	t-critical(0.95;132):	1.969
Durbin-Watson Factor:	4.122		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.33	132	Fn					
1	s:	1.38	1.34	131	Cn B					
2	s:	1.45	1.33	133	F2					
3	s:	1.47	1.33	132	C1 B					
4	s:	2.55	1.33	133	B1					
5	s:	3.37	1.33	132	An					
6	s:	5.06	1.33	133	A3					
7	s:	6.19	1.33	133	A2					
8	s:	9.01	1.33	133	F1					
9	s:	17.21	1.33	133	R3					
10	s:	20.78	1.33	133	D1F					
11	s:	21.92	1.33	133	D3F					
12	s:	22.44	1.33	133	D3					
13	s:	23.74	1.33	133	R2					
14	s:	33.92	1.33	133	D4					
15	s:	45.17	1.33	133	D2					
16	s:	68.19	1.33	133	D1					
17	s:	1856.75	1.28	261	Bna					

Sample 11 / cycle 13 / Fn

NETZSCH Thermokinetics
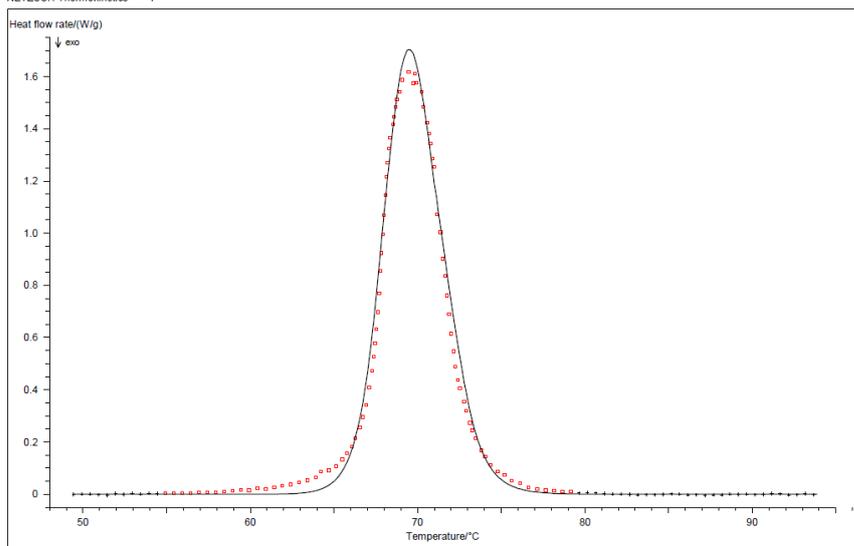
Date/Time: 30.11.2016 at 15:02

Project: 1
Model   1: n-th order   A—1→B

Start evaluation:	0.00050	Measurement type: DSC
Fine evaluation:	0.99950	
SCAN 1 Identity:		OP320 27.04.2016 17:04:37/Segm.S2/3
Transfer Corr:	204 F1.kcr	
Min. Temp/°C:	49.4455	Min. Time/min: 0.0
Max. Temp°C:	93.8708	Max. Time/min: 4.9533
Heating rate/(K/min):	8.969	Sampling time/s: 0.669
Sample mass/mg:	3.770	
Base line type:		LeftPts: 20 RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	170.2299	170.1915				4.9039E-2
1	E1 kJ/mol	1121.5213	1121.2698			+	0.3605
2	React.ord. 1	2.3538	2.3530			+	7.2426E-2
3	Area 1/(J/g)	52.4495	52.4495				constant

STATISTICS

Least squares:	5.79244	Number of cycles:	2
Mean of residues:	0.11409	Max.No of cycles:	50
Correlation coefficient:	0.995732	Rel. precision:	0.001000
Durbin-Watson Value:	0.093	t-critical(0.95;246):	1.961
Durbin-Watson Factor:	3.312		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.24	245	Cn B					
1	s:	1.02	1.24	247	B1					
2	s:	1.04	1.24	246	C1 B					
3	s:	1.25	1.24	246	Fn					
4	s:	1.40	1.24	247	F2					
5	s:	3.64	1.24	246	An					
6	s:	3.72	1.24	247	A3					
7	s:	4.05	1.24	247	A2					
8	s:	5.47	1.24	247	F1					
9	s:	10.14	1.24	247	R3					
10	s:	11.51	1.24	247	D1F					
11	s:	12.64	1.24	247	D3F					
12	s:	13.16	1.24	247	D3					
13	s:	13.97	1.24	247	R2					
14	s:	20.19	1.24	247	D4					
15	s:	26.71	1.24	247	D2					
16	s:	41.24	1.24	247	D1					
17	s:	3029.18	1.23	261	Bna					

Sample 11 / cycle 14 / Fn
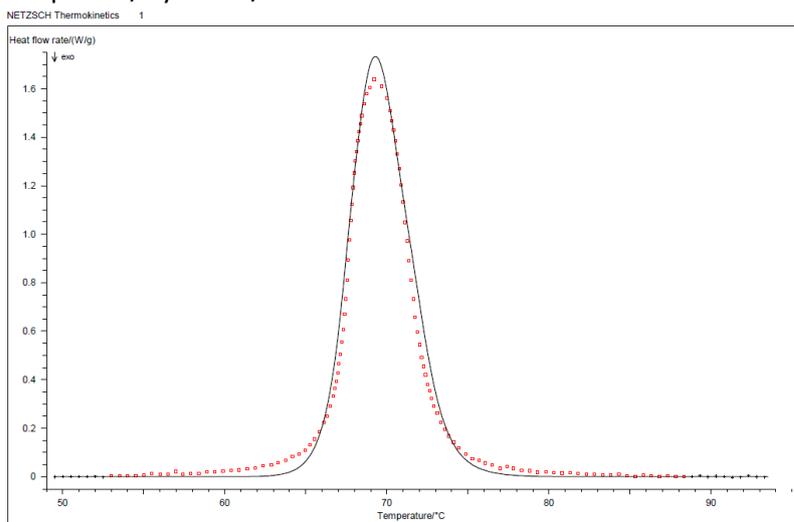
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 15:09

Project: 1
Model 1: n-th order

A—1→B

Start evaluation:	0.00050	Measurement type: DSC
Fine evaluation:	0.99950	
SCAN 1 Identity:		OP320 27.04.2016 17:44:40/Segm.S2/3
Transfer Corr:	204 F1.kcr	
Min. Temp/°C:	49.5091	Min. Time/min: 0.0
Max. Temp°C:	93.5203	Max. Time/min: 4.9104
Heating rate/(K/min):	8.963	Sampling time/s: 0.670
Sample mass/mg:	3.770	
Base line type:	tangent area prop.	LeftPts: 10 RightPts: 10

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	172.0402	172.0402				1.8948E-2
1	E1 kJ/mol	1132.6281	1132.6281			+	0.2282
2	React.ord. 1	2.4906	2.4906			+	0.1142
3	Area 1/(J/g)	54.8202	54.8202				constant

STATISTICS

Least squares:	8.71146	Number of cycles:	14
Mean of residues:	0.14055	Max.No of cycles:	50
Correlation coefficient:	0.994406	Rel. precision:	0.001000
Durbin-Watson Value:	0.027	t-critical(0.95;358):	1.958
Durbin-Watson Factor:	6.099		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.19	357	Cn B					
1	s:	1.17	1.19	359	B1					
2	s:	1.22	1.19	358	C1 B					
3	s:	1.60	1.19	358	Fn					
4	s:	1.83	1.19	359	F2					
5	s:	3.80	1.19	358	An					
6	s:	3.94	1.19	359	A3					
7	s:	4.29	1.19	359	A2					
8	s:	5.64	1.19	359	F1					
9	s:	9.81	1.19	359	R3					
10	s:	10.61	1.19	359	D1F					
11	s:	11.93	1.19	359	D3F					
12	s:	12.53	1.19	359	D3					
13	s:	13.17	1.19	359	R2					
14	s:	18.63	1.19	359	D4					
15	s:	24.76	1.19	359	D2					
16	s:	36.15	1.19	359	D1					
17	s:	3746.33	1.21	261	Bna					

Sample 11 / cycle 15 / Fn

NETZSCH Thermokinetics   1
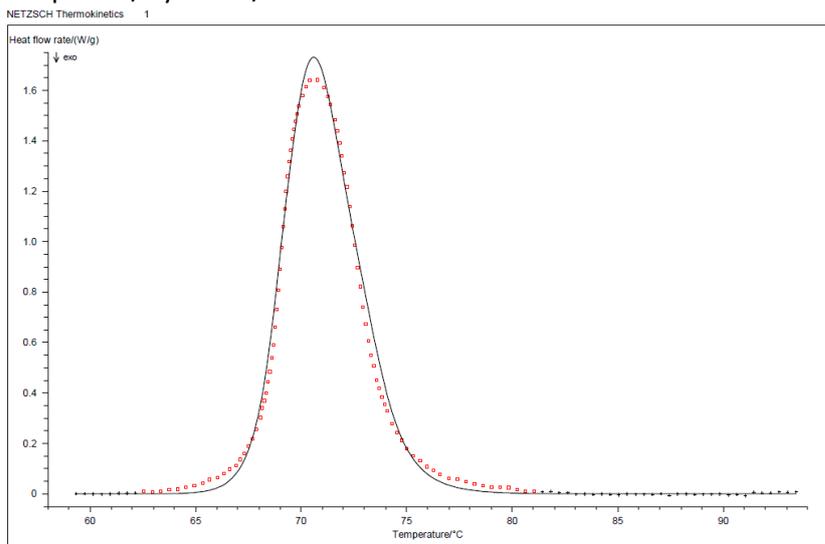
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 15:13

Project: 1
Model   1: n-th order

A —1→ B

Start evaluation:	0.00050	Measurement type: DSC
Fine evaluation:	0.99950	
SCAN 1 Identity:		OP320 28.04.2016 12:45:11/Segm.S2/3
Transfer Corr:	204 F1.kcr	
Min. Temp/°C:	59.3390	Min. Time/min: 0.0
Max. Temp°C:	93.4503	Max. Time/min: 3.7967
Heating rate/(K/min):	8.985	Sampling time/s: 0.670
Sample mass/mg:	3.770	
Base line type:	tangent area prop.	LeftPts: 15 RightPts: 113

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	146.8558	197.8545				0.1212
1	E1 kJ/mol	972.0876	1306.3093			+	0.8383
2	React.ord. 1	2.1064	2.7619			+	7.7462E-2
3	Area 1/(J/g)	51.5313	51.5313				constant

STATISTICS

Least squares:	5.42073	Number of cycles:	8
Mean of residues:	0.12608	Max.No of cycles:	50
Correlation coefficient:	0.996655	Rel. precision:	0.001000
Durbin-Watson Value:	0.044	t-critical(0.95;187):	1.964
Durbin-Watson Factor:	4.802		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.28	186	Cn B					
1	s:	1.04	1.27	187	Fn					
2	s:	1.07	1.27	188	B1					
3	s:	1.09	1.27	187	C1 B					
4	s:	1.71	1.27	188	F2					
5	s:	4.16	1.27	187	An					
6	s:	5.82	1.27	188	A2					
7	s:	7.91	1.27	188	F1					
8	s:	14.10	1.27	188	R3					
9	s:	16.20	1.27	188	D1F					
10	s:	17.49	1.27	188	D3F					
11	s:	18.07	1.27	188	D3					
12	s:	18.95	1.27	188	R2					
13	s:	27.01	1.27	188	D4					
14	s:	33.59	1.27	188	D2					
15	s:	40.37	1.27	188	A3					
16	s:	50.67	1.27	188	D1					
17	s:	2048.47	1.25	261	Bna					

Sample 11 / cycle 16 / Fn

NETZSCH Thermokinetics   1
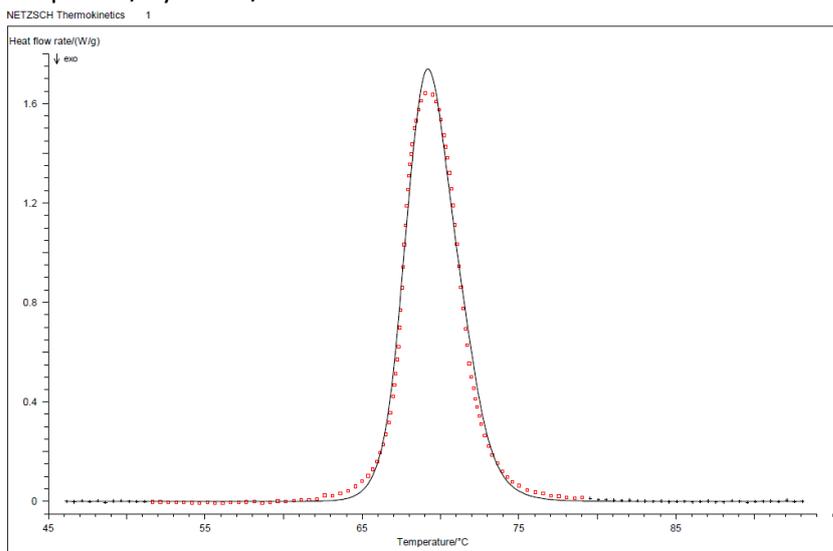
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 15:20

Project: 1
Model   1: n-th order

A—1→B

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 28.04.2016 13:26:28/Segm.S2/3	
Transfer Corr:	204 F1.kcr		
Min. Temp/°C:	46.1494	Min. Time/min:	0.0
Max. Temp°C:	93.1656	Max. Time/min:	5.2446
Heating rate/(K/min):	8.965	Sampling time/s:	0.670
Sample mass/mg:	3.770		
Base line type:	tangent area prop.	LeftPts: 10	RightPts: 11

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	132.5011	192.8504				1.5159E-2
1	E1 kJ/mol	874.3818	1268.3211			+	0.1993
2	React.ord. 1	1.8602	2.5705			+	0.1021
3	Area 1/(J/g)	50.5800	50.5800				constant

STATISTICS

Least squares:	3.76645	Number of cycles:	23
Mean of residues:	8.94244E-2	Max.No of cycles:	50
Correlation coefficient:	0.997307	Rel. precision:	0.001000
Durbin-Watson Value:	0.059	t-critical(0.95;276):	1.960
Durbin-Watson Factor:	4.131		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.22	276	Fn					
1	s:	1.41	1.22	277	F2					
2	s:	1.43	1.22	275	Cn B					
3	s:	1.65	1.22	276	C1 B					
4	s:	4.86	1.22	276	An					
5	s:	4.86	1.22	277	A3					
6	s:	5.20	1.22	277	A2					
7	s:	7.05	1.22	277	F1					
8	s:	13.07	1.22	277	R3					
9	s:	15.74	1.22	277	D1F					
10	s:	16.64	1.22	277	D3F					
11	s:	17.04	1.22	277	D3					
12	s:	17.98	1.22	277	R2					
13	s:	25.59	1.22	277	D4					
14	s:	26.50	1.22	277	B1					
15	s:	35.94	1.22	277	D2					
16	s:	54.49	1.22	277	D1					
17	s:	4167.09	1.22	261	Bna					

Sample 11 / cycle 17 / Fn

NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 15:22

Project: 1
Model 1: n-th order

$A \longrightarrow 1 \rightarrow B$

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP320 28.04.2016 16:37:10/Segm.S1/2		
Transfer Corr:	204 F1.kcr			
Min. Temp/°C:	57.8795	Min. Time/min:		0.0
Max. Temp°C:	90.0545	Max. Time/min:		3.5880
Heating rate/(K/min):	8.967	Sampling time/s:		0.671
Sample mass/mg:	3.770			
Base line type:	tangent area prop.	LeftPts: 20		RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	143.8968	196.9185				0.2320
1	E1 kJ/mol	951.0432	1297.9341			+	1.5535
2	React.ord. 1	2.0501	2.7130			+	6.8979E-2
3	Area 1/(J/g)	51.0422	51.0422				constant

STATISTICS

Least squares:	5.91356	Number of cycles:	9
Mean of residues:	0.13552	Max.No of cycles:	50
Correlation coefficient:	0.996731	Rel. precision:	0.001000
Durbin-Watson Value:	0.043	t-critical(0.95;212):	1.962
Durbin-Watson Factor:	4.858		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.26	211	Cn B					
1	s:	1.04	1.26	212	Fn					
2	s:	1.10	1.26	212	C1 B					
3	s:	1.60	1.26	213	F2					
4	s:	3.07	1.26	213	B1					
5	s:	4.12	1.26	212	An					
6	s:	5.41	1.26	213	A2					
7	s:	7.34	1.26	213	F1					
8	s:	13.17	1.26	213	R3					
9	s:	15.26	1.26	213	D1F					
10	s:	16.46	1.26	213	D3F					
11	s:	16.98	1.26	213	D3					
12	s:	17.78	1.26	213	R2					
13	s:	25.37	1.26	213	D4					
14	s:	31.63	1.26	213	D2					
15	s:	42.18	1.26	213	A3					
16	s:	48.47	1.26	213	D1					
17	s:	2115.15	1.24	261	Bna					

Sample 12 / cycle 1 / Fn

NETZSCH Thermokinetics   1

Heat flow rate/(W/g)
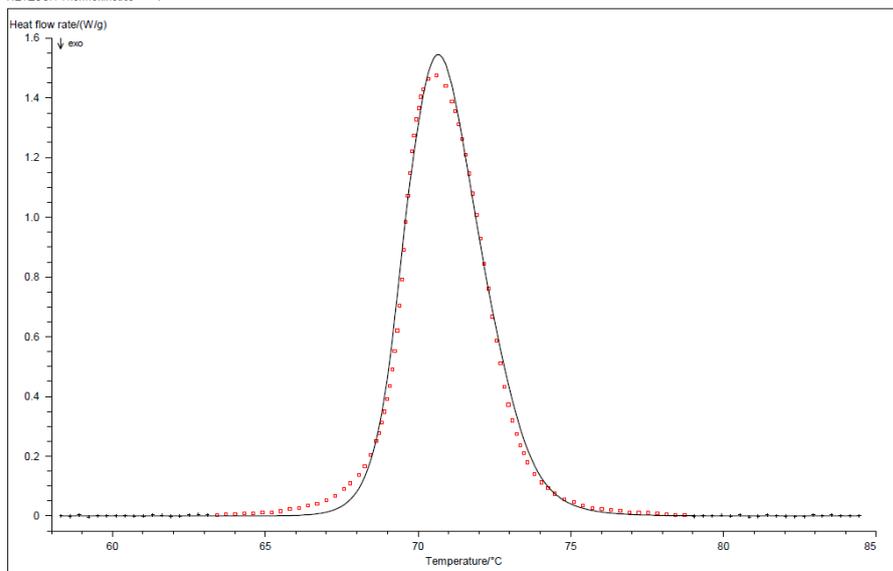
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Project: 1
Model 1: n-th order   A—1→B

Start evaluation: 0.00050   Measurement type: DSC
Fine evaluation: 0.99950
SCAN 1   Identity: OP320 08.05.2016 16:43:02/Segm.S2/3
Transfer Corr: 204 F1.kcr
Min. Temp/°C: 58.3092   Min. Time/min: 0.0
Max. Temp°C: 84.4382   Max. Time/min: 4.3684
Heating rate/(K/min):   5.981   Sampling time/s: 1.004
Sample mass/mg: 3.580
Base line type: tangent area prop. LeftPts: 40   RightPts: 40

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	240.0272	275.7141				8.1325E-2
1	E1 kJ/mol	1584.5552	1818.9149			+	0.5907
2	React.ord. 1	2.4714	2.7588			+	8.6118E-2
3	Area 1/(J/g)	51.2602	51.2602				constant

STATISTICS
Least squares: 3.72775   Number of cycles: 9
Mean of residues: 0.11928   Max.No of cycles: 50
Correlation coefficient: 0.997215   Rel. precision: 0.001000
Durbin-Watson Value: 0.065   t-critical(0.95;153):   1.967
Durbin-Watson Factor: 3.951

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.31	152	Cn B					
1	s:	1.01	1.31	154	B1					
2	s:	1.06	1.31	153	Fn					
3	s:	1.15	1.31	153	C1 B					
4	s:	1.80	1.31	154	F2					
5	s:	4.83	1.28	212	An					
6	s:	5.19	1.31	154	A3					
7	s:	5.92	1.31	154	A2					
8	s:	8.90	1.31	154	F1					
9	s:	16.28	1.31	154	R3					
10	s:	19.45	1.31	154	D1F					
11	s:	21.57	1.31	154	D3F					
12	s:	22.20	1.31	154	R2					
13	s:	22.32	1.31	154	D3					
14	s:	32.38	1.31	154	D4					
15	s:	40.59	1.31	154	D2					
16	s:	62.03	1.31	154	D1					
17	s:	2479.42	1.26	261	Bna					

Sample 12 / cycle 2 / Fn

NETZSCH Thermokinetics
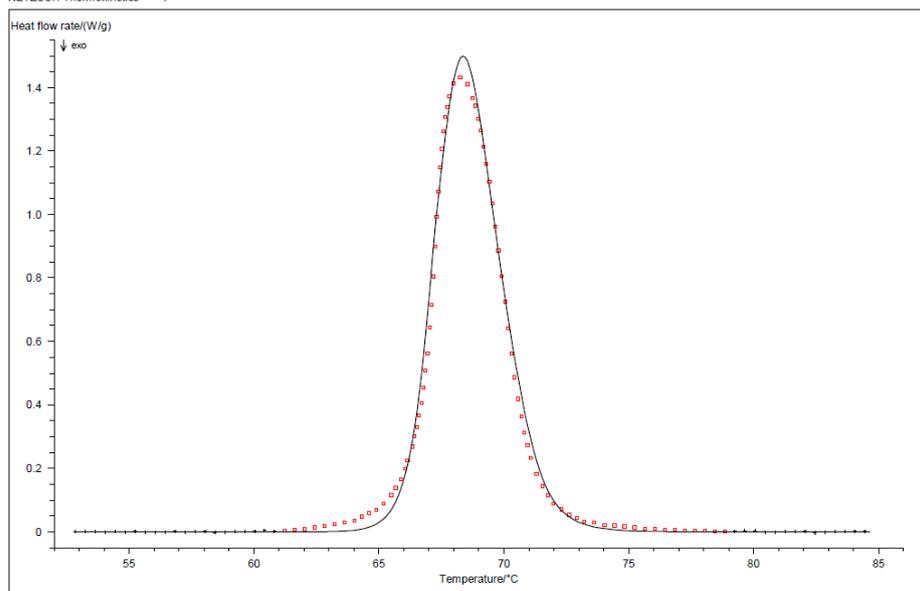
Date/Time: 30.11.2016 at 15:40

Project: 1
Model   1: n-th order

A—1→B

Start evaluation:	0.00050	Measurement type: DSC
Fine evaluation:	0.99950	
SCAN 1 Identity:		OP320 08.05.2016 17:31:51/Segm.S2/3
Transfer Corr:	204_F1.kcr	
Min. Temp/°C:	52.8310	Min. Time/min: 0.0
Max. Temp°C:	84.6507	Max. Time/min: 5.3233
Heating rate/(K/min):	5.977	Sampling time/s: 1.004
Sample mass/mg:	3.510	
Base line type:	tangent area prop.	LeftPts: 25 RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	256.0020	256.0020				2.0582E-2
1	E1 kJ/mol	1678.2027	1678.2027			+	0.3908
2	React.ord. 1	2.6590	2.6590			+	0.2007
3	Area 1/(J/g)	50.9277	50.9277				constant

STATISTICS

Least squares:	3.36762	Number of cycles:	14
Mean of residues:	0.10275	Max.No of cycles:	50
Correlation coefficient:	0.996909	Rel. precision:	0.001000
Durbin-Watson Value:	0.059	t-critical(0.95;174):	1.965
Durbin-Watson Factor:	4.135		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.28	175	B1					
1	s:	1.03	1.29	173	Cn B					
2	s:	1.20	1.29	174	Fn					
3	s:	1.30	1.29	174	C1 B					
4	s:	1.77	1.28	175	F2					
5	s:	5.76	1.28	175	A2					
6	s:	8.40	1.28	175	F1					
7	s:	11.49	1.28	175	A3					
8	s:	15.48	1.28	175	R3					
9	s:	18.13	1.28	175	D1F					
10	s:	20.15	1.28	175	D3F					
11	s:	20.87	1.28	175	D3					
12	s:	21.17	1.28	175	R2					
13	s:	31.93	1.28	175	D4					
14	s:	38.47	1.28	175	D2					
15	s:	58.27	1.28	175	D1					
16	s:	210.55	1.29	174	An					
17	s:	3533.72	1.25	261	Bna					

Sample 12 / cycle 3 / Fn

NETZSCH Thermokinetics
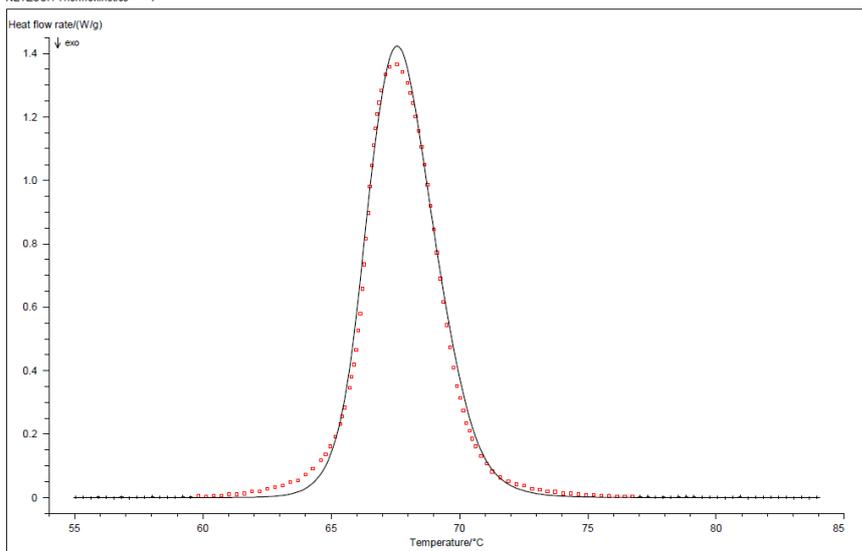
Date/Time: 30.11.2016 at 15:42

Project: 1
Model   1: n-th order

A—1→B

Start evaluation:		0.00050	Measurement type:	DSC
Fine evaluation:		0.99950		
SCAN 1	Identity:		OP320 08.05.2016 18:14:53/Segm.S2/3	
Transfer Corr:		204 F1.kcr		
Min. Temp/°C:		55.0315	Min. Time/min:	0.0
Max. Temp°C:		84.0442	Max. Time/min:	4.8542
Heating rate/(K/min):		5.977	Sampling time/s:	1.004
Sample mass/mg:		3.510		
Base line type:	tangent area prop.		LeftPts: 25	RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	236.7421	236.7421				1.9547E-2
1	E1 kJ/mol	1548.9595	1548.9595			+	0.3543
2	React.ord. 1	2.5192	2.5192			+	0.1805
3	Area 1/(J/g)	49.5824	49.5824				constant

STATISTICS

Least squares:	2.95990	Number of cycles:	14
Mean of residues:	0.10085	Max.No of cycles:	50
Correlation coefficient:	0.997280	Rel. precision:	0.001000
Durbin-Watson Value:	0.057	t-critical(0.95;171):	1.965
Durbin-Watson Factor:	4.236		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.29	172	B1					
1	s:	1.10	1.29	170	Cn B					
2	s:	1.12	1.29	171	C1 B					
3	s:	1.27	1.29	171	Fn					
4	s:	1.75	1.29	172	F2					
5	s:	5.40	1.29	171	An					
6	s:	6.56	1.29	172	A2					
7	s:	9.44	1.29	172	F1					
8	s:	17.94	1.29	172	R3					
9	s:	20.85	1.29	172	D1F					
10	s:	23.03	1.29	172	D3F					
11	s:	23.84	1.29	172	D3					
12	s:	24.80	1.29	172	R2					
13	s:	35.80	1.29	172	D4					
14	s:	45.95	1.29	172	D2					
15	s:	69.70	1.29	172	D1					
16	s:	331.91	1.29	172	A3					
17	s:	4186.85	1.25	261	Bna					

Sample 12 / cycle 4 / Fn

NETZSCH Thermokinetics
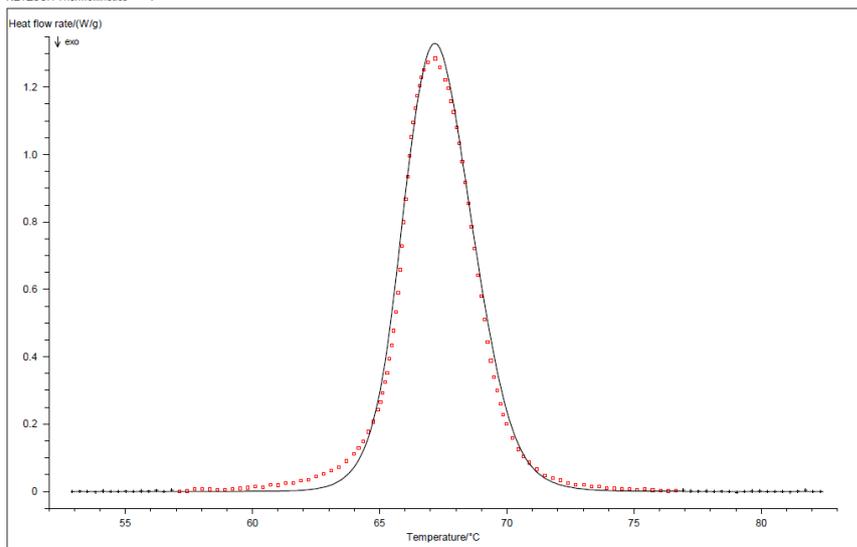
Date/Time: 30.11.2016 at 15:50

Project: 1
Model   1: n-th order

$A \xrightarrow{1} B$

Start evaluation:	0.00050	Measurement type: DSC
Fine evaluation:	0.99950	
SCAN 1 Identity:		OP320 08.05.2016 18:56:23/Segm.S2/3
Transfer Corr:	204 F1.kcr	
Min. Temp/°C:	52.9259	Min. Time/min: 0.0
Max. Temp°C:	82.4358	Max. Time/min: 4.9387
Heating rate/(K/min):	5.975	Sampling time/s: 1.004
Sample mass/mg:	3.590	
Base line type:	tangent area prop.	LeftPts: 25 RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	214.3131	214.3131				1.9397E-2
1	E1 kJ/mol	1401.4228	1401.4228			+	0.3378
2	React.ord. 1	2.3296	2.3296			+	0.1687
3	Area 1/(J/g)	47.8813	47.8813				constant

STATISTICS

Least squares:	2.82774	Number of cycles:	14
Mean of residues:	9.77403E-2	Max.No of cycles:	50
Correlation coefficient:	0.997143	Rel. precision:	0.001000
Durbin-Watson Value:	0.040	t-critical(0.95;195):	1.963
Durbin-Watson Factor:	5.023		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.27	196	B1					
1	s:	1.14	1.27	194	Cn B					
2	s:	1.51	1.27	195	C1 B					
3	s:	1.61	1.27	195	Fn					
4	s:	1.85	1.27	196	F2					
5	s:	5.83	1.27	195	An					
6	s:	6.92	1.27	196	A2					
7	s:	9.79	1.27	196	F1					
8	s:	19.23	1.27	196	R3					
9	s:	21.72	1.27	196	D1F					
10	s:	24.23	1.27	196	D3F					
11	s:	25.24	1.27	196	D3					
12	s:	26.91	1.27	196	R2					
13	s:	34.26	1.27	196	A3					
14	s:	39.96	1.27	196	D4					
15	s:	51.27	1.27	196	D2					
16	s:	79.56	1.27	196	D1					
17	s:	6308.39	1.25	261	Bna					

Sample 12 / cycle 5 / Fn

NETZSCH Thermokinetics   1
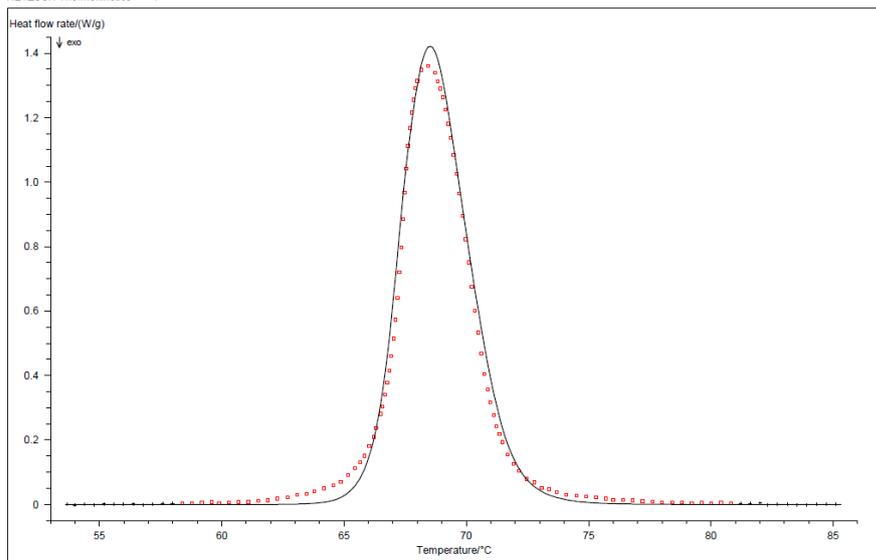
NETZSCH Thermokinetics　　　　　　　　　Date/Time: 30.11.2016 at 15:52

Project: 1
Model   1: n-th order　　　　　　　　　　　A—1→B

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 10.05.2016 11:06:30/Segm.S2/3	
Transfer Corr:	204 F1.kcr		
Min. Temp/°C:	53.6883	Min. Time/min:	0.0
Max. Temp°C:	85.3150	Max. Time/min:	5.2941
Heating rate/(K/min):	5.974	Sampling time/s:	1.005
Sample mass/mg:	3.590		
Base line type:	tangent area prop.	LeftPts: 25	RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	247.1558	247.1558				2.1389E-2
1	E1 kJ/mol	1621.1392	1621.1392			+	0.3714
2	React.ord. 1	2.7046	2.7046			+	0.1934
3	Area 1/(J/g)	50.2719	50.2719				constant

STATISTICS

Least squares:	4.51392	Number of cycles:	14
Mean of residues:	0.11933	Max.No of cycles:	50
Correlation coefficient:	0.995776	Rel. precision:	0.001000
Durbin-Watson Value:	0.038	t-critical(0.95;224):	1.962
Durbin-Watson Factor:	5.146		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.25	223	Cn B					
1	s:	1.32	1.25	224	C1 B					
2	s:	2.03	1.25	224	Fn					
3	s:	2.76	1.25	225	F2					
4	s:	6.24	1.25	224	An					
5	s:	7.41	1.25	225	A2					
6	s:	10.47	1.25	225	F1					
7	s:	18.56	1.25	225	R3					
8	s:	20.17	1.25	225	B1					
9	s:	20.70	1.25	225	D1F					
10	s:	23.53	1.25	225	D3F					
11	s:	24.58	1.25	225	D3					
12	s:	25.00	1.25	225	R2					
13	s:	36.55	1.25	225	D4					
14	s:	44.94	1.25	225	D2					
15	s:	67.46	1.25	225	D1					
16	s:	314.24	1.25	225	A3					
17	s:	993.11	1.25	223	Bna					

Sample 12 / cycle 6 / Fn
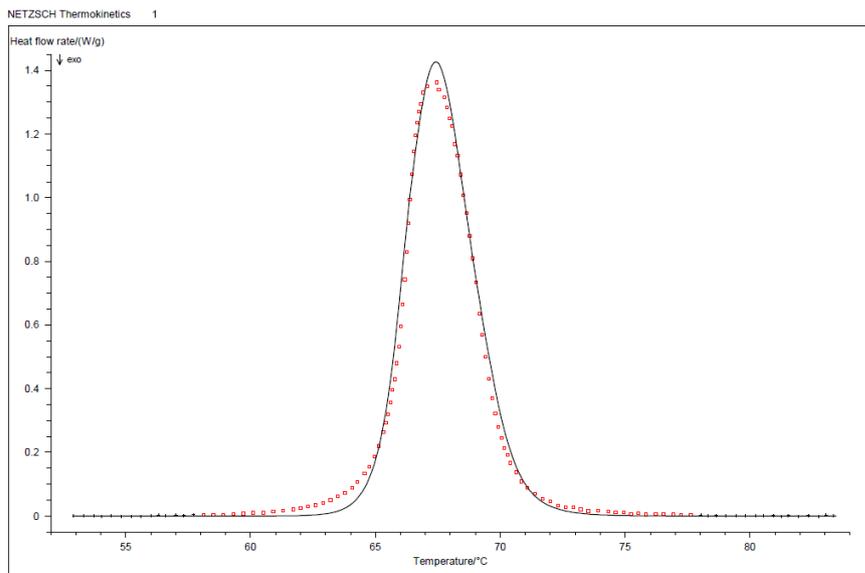
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 15:54

Project: 1
Model 1: n-th order

A—1→B

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP320 10.05.2016 12:19:04/Segm.S2/3		
Transfer Corr:	204 F1.kcr			
Min. Temp/°C:	52.9196	Min. Time/min:		0.0
Max. Temp°C:	83.4344	Max. Time/min:		5.1066
Heating rate/(K/min):	5.976	Sampling time/s:		1.005
Sample mass/mg:	3.590			
Base line type:	tangent area prop.	LeftPts: 25		RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	239.4723	239.4723				2.1819E-2
1	E1 kJ/mol	1565.9649	1565.9649			+	0.3987
2	React.ord. 1	2.5355	2.5355			+	0.2034
3	Area 1/(J/g)	49.5771	49.5771				constant

STATISTICS

Least squares:	4.01552	Number of cycles:	14
Mean of residues:	0.11455	Max.No of cycles:	50
Correlation coefficient:	0.996248	Rel. precision:	0.001000
Durbin-Watson Value:	0.059	t-critical(0.95;194):	1.963
Durbin-Watson Factor:	4.148		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.27	195	B1					
1	s:	1.08	1.27	194	C1 B					
2	s:	1.13	1.27	193	Cn B					
3	s:	1.56	1.27	194	Fn					
4	s:	1.97	1.27	195	F2					
5	s:	4.87	1.27	194	An					
6	s:	5.76	1.27	195	A2					
7	s:	8.33	1.27	195	F1					
8	s:	15.40	1.27	195	R3					
9	s:	17.75	1.27	195	D1F					
10	s:	19.88	1.27	195	D3F					
11	s:	20.65	1.27	195	D3					
12	s:	21.07	1.27	195	R2					
13	s:	30.78	1.27	195	D4					
14	s:	39.19	1.27	195	D2					
15	s:	59.61	1.27	195	D1					
16	s:	281.32	1.27	195	A3					
17	s:	742.06	1.26	223	Bna					

Sample 12 / cycle 7 / Fn

NETZSCH Thermokinetics   1
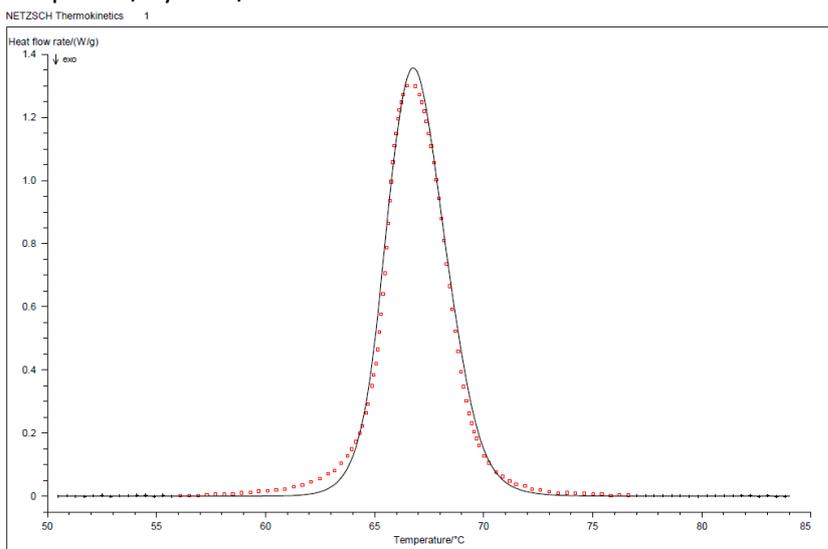
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 15:56

Project: 1
Model   1: n-th order

A—1→B

Start evaluation:	0.00050	Measurement type: DSC
Fine evaluation:	0.99950	
SCAN 1 Identity:		OP320 10.05.2016 13:07:36/Segm.S2/3
Transfer Corr:	204 F1.kcr	
Min. Temp/°C:	50.5080	Min. Time/min: 0.0
Max. Temp°C:	84.0191	Max. Time/min: 5.6093
Heating rate/(K/min):	5.974	Sampling time/s: 1.005
Sample mass/mg:	3.590	
Base line type:	tangent area prop.	LeftPts: 25 RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	224.3049	217.2666				0.3045
1	E1 kJ/mol	1464.2291	1418.9183			+	2.0169
2	React.ord. 1	2.5272	2.3496			+	7.1785E-2
3	Area 1/(J/g)	48.6399	48.6399				constant

STATISTICS

Least squares:	3.12527	Number of cycles:	9
Mean of residues:	9.64438E-2	Max.No of cycles:	50
Correlation coefficient:	0.996570	Rel. precision:	0.001000
Durbin-Watson Value:	0.040	t-critical(0.95;204):	1.963
Durbin-Watson Factor:	5.052		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.26	205	B1					
1	s:	1.06	1.26	204	C1 B					
2	s:	1.10	1.26	203	Cn B					
3	s:	1.71	1.26	204	Fn					
4	s:	1.94	1.26	205	F2					
5	s:	5.38	1.26	204	An					
6	s:	5.58	1.26	205	A3					
7	s:	6.21	1.26	205	A2					
8	s:	8.83	1.26	205	F1					
9	s:	16.98	1.26	205	R3					
10	s:	19.11	1.26	205	D1F					
11	s:	21.49	1.26	205	D3F					
12	s:	22.44	1.26	205	D3					
13	s:	24.08	1.26	205	R2					
14	s:	35.41	1.26	205	D4					
15	s:	44.59	1.26	205	D2					
16	s:	68.44	1.26	205	D1					
17	s:	1102.13	1.25	223	Bna					

Sample 12 / cycle 8 / Fn
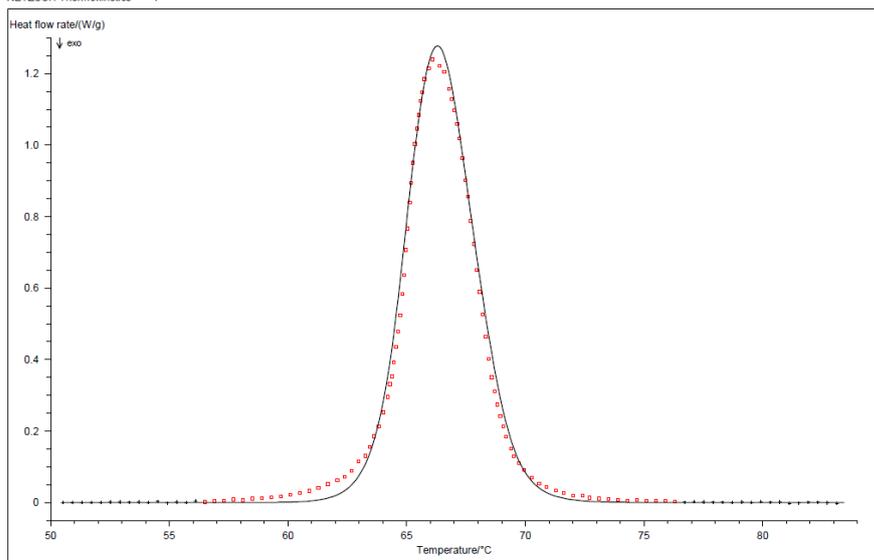
NETZSCH Thermokinetics   Date/Time: 30.11.2016 at 15:58

Project: 1
Model   1: n-th order   A—1→B

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP320 10.05.2016 13:49:34/Segm.S2/3		
Transfer Corr.:	204 F1.kcr			
Min. Temp°C:	50.5127	Min. Time/min:		0.0
Max. Temp°C:	83.4191	Max. Time/min:		5.5095
Heating rate/(K/min):	5.973	Sampling time/s:		1.005
Sample mass/mg:	3.590			
Base line type:	tangent area prop.	LeftPts: 35		RightPts: 35

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	197.7118	197.7119				2.2433E-2
1	E1 kJ/mol	1290.2549	1290.2549			+	0.2035
2	React.ord. 1	2.2047	2.2050			+	8.0337E-2
3	Area 1/(J/g)	47.3854	47.3854				constant

STATISTICS

Least squares:	2.52075	Number of cycles:	14
Mean of residues:	8.73993E-2	Max.No of cycles:	50
Correlation coefficient:	0.996981	Rel. precision:	0.001000
Durbin-Watson Value:	0.044	t-critical(0.95;200):	1.963
Durbin-Watson Factor:	4.806		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.26	201	B1					
1	s:	1.05	1.26	200	C1 B					
2	s:	1.09	1.26	199	Cn B					
3	s:	1.76	1.26	200	Fn					
4	s:	1.86	1.26	201	F2					
5	s:	5.81	1.26	200	An					
6	s:	6.71	1.26	201	A2					
7	s:	9.34	1.26	201	F1					
8	s:	14.52	1.26	201	A3					
9	s:	18.82	1.26	201	R3					
10	s:	20.90	1.26	201	D1F					
11	s:	23.39	1.26	201	D3F					
12	s:	24.43	1.26	201	D3					
13	s:	26.76	1.26	201	R2					
14	s:	38.32	1.26	201	D4					
15	s:	52.34	1.26	201	D2					
16	s:	78.81	1.26	201	D1					
17	s:	1378.01	1.25	223	Bna					

Sample 12 / cycle 9 / Fn

NETZSCH Thermokinetics   1
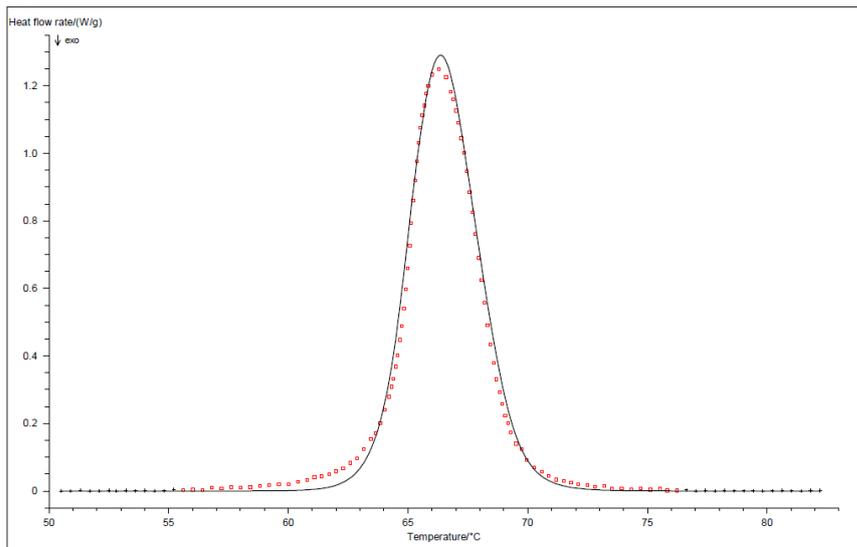
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 16:00

Project: 1
Model   1: n-th order

A—1→B

Start evaluation: 0.00050
Fine evaluation: 0.99950
SCAN 1   Identity:
Transfer Corr: 204 F1.kcr
Min. Temp/°C: 50.5146
Max. Temp°C: 82.2246
Heating rate/(K/min):   5.975
Sample mass/mg: 3.590
Base line type: tangent area prop.

Measurement type: DSC

OP320 10.05.2016 14:30:57/Segm.S2/3

Min. Time/min: 0.0
Max. Time/min: 5.3067
Sampling time/s: 1.004

LeftPts: 25   RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	200.5088	200.5088				2.0934E-2
1	E1 kJ/mol	1308.6182	1308.6182			+	0.3527
2	React.ord. 1	2.2205	2.2205			+	0.1741
3	Area 1/(J/g)	47.5906	47.5906				constant

STATISTICS

Least squares:	3.04965	Number of cycles:	14
Mean of residues:	9.79290E-2	Max.No of cycles:	50
Correlation coefficient:	0.996565	Rel. precision:	0.001000
Durbin-Watson Value:	0.033	t-critical(0.95;208):	1.963
Durbin-Watson Factor:	5.501		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.26	207	Cn B					
1	s:	1.12	1.26	209	B1					
2	s:	1.15	1.26	208	C1 B					
3	s:	2.11	1.26	208	Fn					
4	s:	2.23	1.26	209	F2					
5	s:	6.16	1.26	208	An					
6	s:	6.44	1.26	209	A3					
7	s:	7.16	1.26	209	A2					
8	s:	10.01	1.26	209	F1					
9	s:	19.79	1.26	209	R3					
10	s:	21.80	1.26	209	D1F					
11	s:	24.61	1.26	209	D3F					
12	s:	25.78	1.26	209	D3					
13	s:	27.87	1.26	209	R2					
14	s:	40.15	1.26	209	D4					
15	s:	52.92	1.26	209	D2					
16	s:	82.20	1.26	209	D1					
17	s:	1418.79	1.25	223	Bna					

Sample 13 / cycle 1 / Fn

NETZSCH Thermokinetics
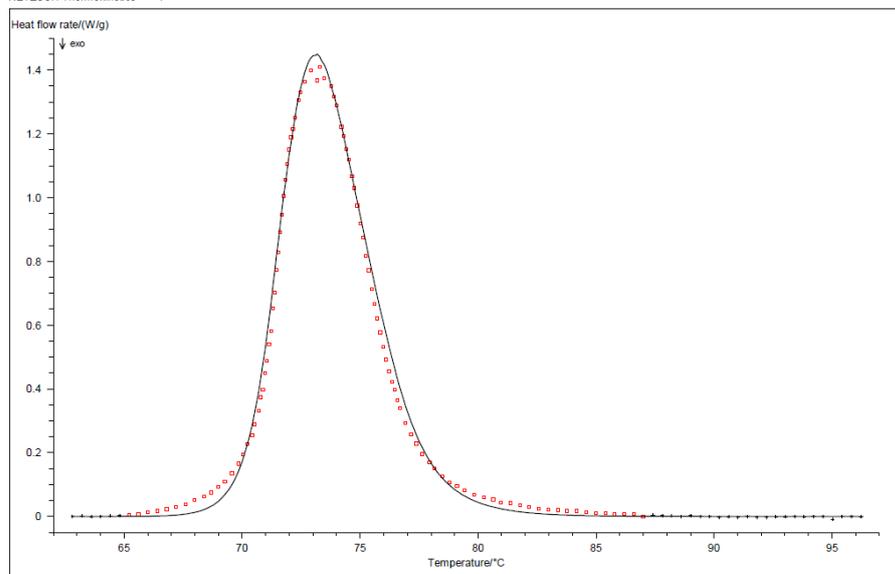
Date/Time: 30.11.2016 at 16:15

Project: 1
Model   1: n-th order

A—1→B

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 27.06.2016 15:34:13/Segm.S1/3
Transfer Corr:	204 F1.kcr		
Min. Temp/°C:	62.8057	Min. Time/min:	0.0
Max. Temp°C:	96.3237	Max. Time/min:	3.7324
Heating rate/(K/min):	8.980	Sampling time/s:	0.670
Sample mass/mg:	4.100		
Base line type:		LeftPts: 20	RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	192.8752	192.8752				1.5079E-2
1	E1 kJ/mol	1282.9317	1282.9317			+	0.1677
2	React.ord. 1	3.0792	3.0792			+	8.9848E-2
3	Area 1/(J/g)	47.3213	47.3213				constant

STATISTICS

Least squares:	3.13378	Number of cycles:	14
Mean of residues:	9.67191E-2	Max.No of cycles:	50
Correlation coefficient:	0.997554	Rel. precision:	0.001000
Durbin-Watson Value:	0.072	t-critical(0.95;216):	1.962
Durbin-Watson Factor:	3.770		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.25	215	Bna					
1	s:	1.00	1.25	215	Cn B					
2	s:	1.33	1.25	216	Fn					
3	s:	1.37	1.25	216	C1 B					
4	s:	3.24	1.25	217	B1					
5	s:	3.50	1.25	217	F2					
6	s:	7.52	1.25	216	An					
7	s:	10.57	1.25	217	A3					
8	s:	12.38	1.25	217	A2					
9	s:	16.42	1.25	217	F1					
10	s:	28.38	1.25	217	R3					
11	s:	30.89	1.25	217	D1F					
12	s:	33.74	1.25	217	D3F					
13	s:	34.92	1.25	217	D3					
14	s:	37.50	1.25	217	R2					
15	s:	50.81	1.25	217	D4					
16	s:	63.28	1.25	217	D2					
17	s:	92.91	1.25	217	D1					

Sample 13 / cycle 2 / Fn

NETZSCH Thermokinetics   1

NETZSCH Thermokinetics

Project: 1
Model   1: n-th order

Date/Time: 30.11.2016 at 16:18

A—1→B

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 27.06.2016 16:05:07/Segm.S1/3
Transfer Corr:	204 F1.kcr		
Min. Temp/°C:	58.2038	Min. Time/min:	0.0
Max. Temp°C:	88.5867	Max. Time/min:	3.4067
Heating rate/(K/min):	8.918	Sampling time/s:	0.670
Sample mass/mg:	4.100		
Base line type:		LeftPts: 50	RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	172.3340	172.3340				1.9103E-2
1	E1 kJ/mol	1142.7247	1142.7247			+	0.2348
2	React.ord. 1	2.4591	2.4591			+	0.1163
3	Area 1/(J/g)	51.8193	51.8193				constant

STATISTICS

Least squares:	7.03725	Number of cycles:	14
Mean of residues:	0.15165	Max.No of cycles:	50
Correlation coefficient:	0.995945	Rel. precision:	0.001000
Durbin-Watson Value:	0.011	t-critical(0.95;224):	1.962
Durbin-Watson Factor:	9.565		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.25	223	Cn B					
1	s:	1.12	1.25	225	B1					
2	s:	1.15	1.25	224	C1 B					
3	s:	1.37	1.25	223	Bna					
4	s:	1.99	1.25	224	Fn					
5	s:	2.41	1.25	225	F2					
6	s:	5.40	1.25	224	An					
7	s:	6.50	1.25	225	A3					
8	s:	7.43	1.25	225	A2					
9	s:	10.36	1.25	225	F1					
10	s:	19.26	1.25	225	R3					
11	s:	21.04	1.25	225	D1F					
12	s:	23.91	1.25	225	D3F					
13	s:	25.13	1.25	225	D3					
14	s:	26.45	1.25	225	R2					
15	s:	38.02	1.25	225	D4					
16	s:	48.71	1.25	225	D2					
17	s:	73.97	1.25	225	D1					

Sample 13 / cycle 3 / Fn
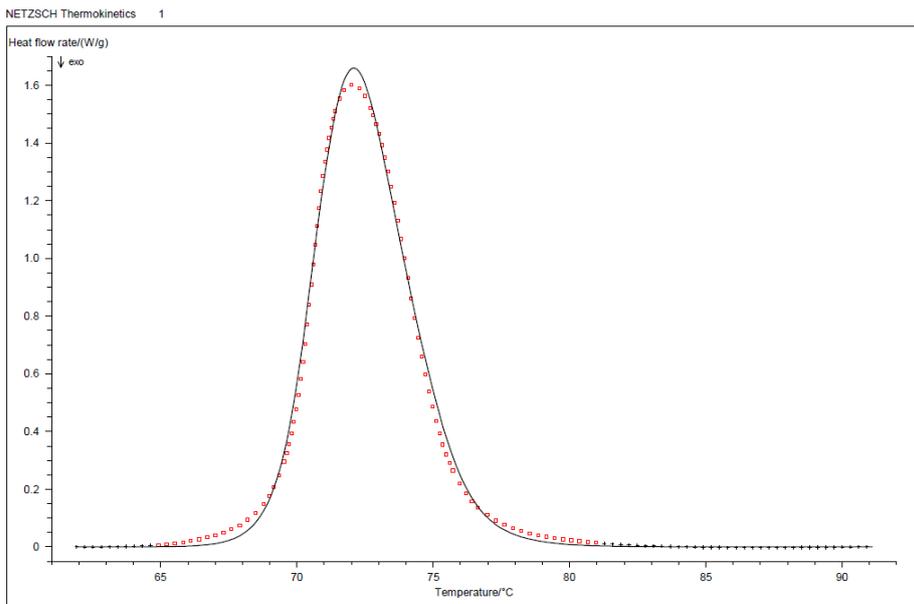
NETZSCH Thermokinetics   Date/Time: 30.11.2016 at 16:22
Project: 1
Model   1: n-th order   A—1→B

Start evaluation: 0.00050   Measurement type: DSC
Fine evaluation: 0.99950
SCAN 1   Identity: OP320 27.06.2016 17:55:36/Segm.S1/3
Transfer Corr: 204 F1.kcr
Min. Temp/°C: 61.9203   Min. Time/min: 0.0
Max. Temp°C: 91.1126   Max. Time/min: 3.2587
Heating rate/(K/min):   8.958   Sampling time/s: 0.672
Sample mass/mg: 4.100
Base line type: LeftPts: 25   RightPts: 50

PARAMETERS AND STANDARD DEVIATIONS

| #	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	160.6675	200.0361				6.3408E-2
1	E1 kJ/mol	1067.1637	1326.3366			+	0.4413
2	React.ord. 1	2.2115	2.6925			+	5.2194E-2
3	Area 1/(J/g)	49.4243	49.4243				constant

STATISTICS
Least squares: 2.75586   Number of cycles: 21
Mean of residues: 9.71487E-2   Max.No of cycles: 50
Correlation coefficient: 0.998330   Rel. precision: 0.001000
Durbin-Watson Value: 0.032   t-critical(0.95;160):   1.966
Durbin-Watson Factor: 5.655

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.30	160	Fn					
1	s:	1.00	1.30	159	Cn B					
2	s:	1.25	1.27	223	Bna					
3	s:	1.64	1.30	161	B1					
4	s:	1.66	1.30	160	C1 B					
5	s:	2.23	1.30	161	F2					
6	s:	6.16	1.30	160	An					
7	s:	10.39	1.30	161	A2					
8	s:	15.25	1.30	161	F1					
9	s:	28.69	1.30	161	R3					
10	s:	33.91	1.30	161	D1F					
11	s:	36.74	1.30	161	D3F					
12	s:	37.87	1.30	161	D3					
13	s:	39.22	1.30	161	R2					
14	s:	53.24	1.30	161	A3					
15	s:	57.10	1.30	161	D4					
16	s:	74.75	1.30	161	D2					
17	s:	106.71	1.30	161	D1					

Sample 13 / cycle 4 / Fn
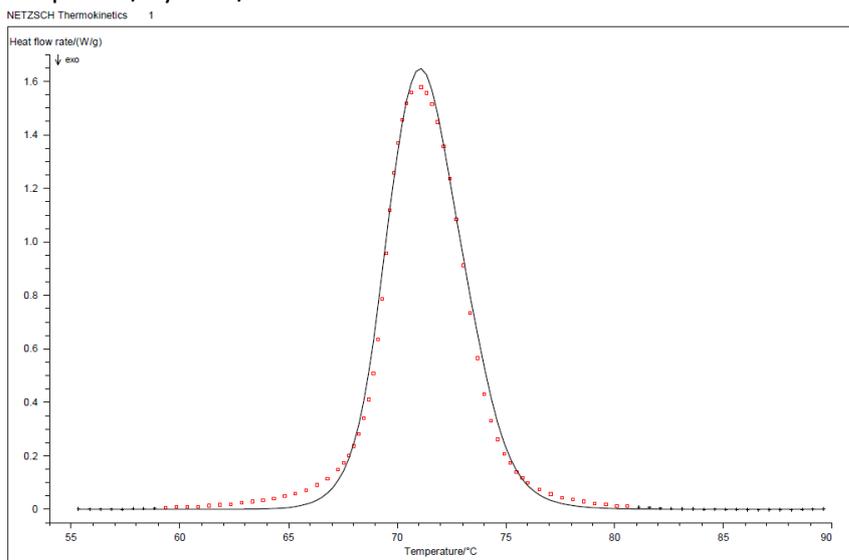
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 16:25

Project: 1
Model   1: n-th order

A—1→B

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 27.06.2016 18:34:46/Segm.S1/3	
Transfer Corr:	204 F1.kcr		
Min. Temp/°C:	55.3493	Min. Time/min:	0.0
Max. Temp°C:	89.6176	Max. Time/min:	3.8303
Heating rate/(K/min):	8.947	Sampling time/s:	1.678
Sample mass/mg:	4.100		
Base line type:		LeftPts: 30	RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	175.3051	175.2992				4.0018E-2
1	E1 kJ/mol	1159.8633	1159.8240			+	0.3392
2	React.ord. 1	2.3936	2.3936			+	0.1218
3	Area 1/(J/g)	50.7611	50.7611				constant

STATISTICS

Least squares:	5.57010	Number of cycles:	1
Mean of residues:	0.20091	Max.No of cycles:	50
Correlation coefficient:	0.996440	Rel. precision:	0.001000
Durbin-Watson Value:	0.111	t-critical(0.95;85):	1.979
Durbin-Watson Factor:	3.041		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.43	86	B1					
1	s:	1.06	1.43	85	C1 B					
2	s:	1.11	1.43	84	Cn B					
3	s:	1.44	1.43	85	Fn					
4	s:	1.68	1.43	86	F2					
5	s:	4.27	1.43	85	An					
6	s:	5.37	1.43	86	A2					
7	s:	7.71	1.43	86	F1					
8	s:	14.72	1.43	86	R3					
9	s:	16.75	1.43	86	D1F					
10	s:	18.75	1.43	86	D3F					
11	s:	19.51	1.43	86	D3					
12	s:	19.76	1.43	86	A3					
13	s:	20.68	1.43	86	R2					
14	s:	29.59	1.43	86	D4					
15	s:	38.00	1.43	86	D2					
16	s:	58.53	1.43	86	D1					
17	s:	365.04	1.43	84	Bna					

Sample 15 / cycle 2 / Fn

NETZSCH Thermokinetics   1
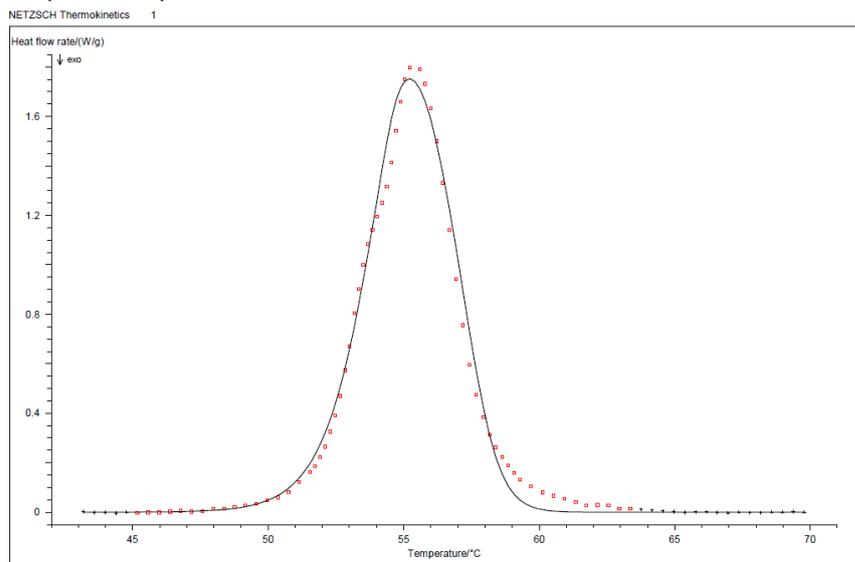
NETZSCH Thermokinetics   Date/Time: 30.11.2016 at 13:16
Project: 1
Model   1: n-th order   A—1→B

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP320 08.04.2016 12:36:46/Segm.S1/3		
Transfer Corr:	204_F1.kcr			
Min. Temp/°C:	43.1838	Min. Time/min:		0.0
Max. Temp°C:	69.7729	Max. Time/min:		2.9724
Heating rate/(K/min):	8.945	Sampling time/s:		1.341
Sample mass/mg:	2.800			
Base line type:		LeftPts: 25	RightPts: 25	

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	127.7227	127.7227				5.1833E-2
1	E1 kJ/mol	808.7707	808.7707			+	0.8107
2	React.ord. 1	1.4790	1.4790			+	0.3518
3	Area 1/(J/g)	50.1979	50.1979				constant

STATISTICS

Least squares:	10.96431	Number of cycles:	14
Mean of residues:	0.28605	Max.No of cycles:	50
Correlation coefficient:	0.994843	Rel. precision:	0.001000
Durbin-Watson Value:	0.161	t-critical(0.95;91):	1.977
Durbin-Watson Factor:	2.544		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.42	90	Cn B					
1	s:	1.11	1.42	91	C1 B					
2	s:	1.26	1.42	91	Fn					
3	s:	1.46	1.42	91	An					
4	s:	1.62	1.42	92	B1					
5	s:	1.65	1.42	92	A3					
6	s:	1.82	1.42	92	A2					
7	s:	1.88	1.42	92	F2					
8	s:	2.31	1.42	92	F1					
9	s:	5.39	1.42	92	R3					
10	s:	5.69	1.42	92	D1F					
11	s:	6.09	1.42	92	D3F					
12	s:	6.67	1.42	92	D3					
13	s:	8.34	1.42	92	R2					
14	s:	11.97	1.42	92	D4					
15	s:	16.86	1.42	92	D2					
16	s:	30.26	1.42	92	D1					

Sample 15 / cycle 3 / Fn

NETZSCH Thermokinetics   Date/Time: 30.11.2016 at 13:19
Project: 1
Model   1: n-th order   A—1→B

Start evaluation: 0.00050   Measurement type: DSC
Fine evaluation: 0.99950
SCAN 1   Identity: OP320 08.04.2016 13:16:26/Segm.S1/3
Transfer Corr: 204_F1.kcr
Min. Temp/°C: 42.3873   Min. Time/min: 0.0
Max. Temp°C: 68.5768   Max. Time/min: 2.9275
Heating rate/(K/min):   8.946   Sampling time/s: 1.341
Sample mass/mg: 2.800
Base line type: LeftPts: 30   RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	123.5428	142.0892				0.7735
1	E1 kJ/mol	782.8291	898.7833			+	4.9433
2	React.ord. 1	1.3845	1.5967			+	0.1120
3	Area 1/(J/g)	51.1564	51.1564				constant

STATISTICS

Least squares:	7.28505	Number of cycles:	8
Mean of residues:	0.23492	Max.No of cycles:	50
Correlation coefficient:	0.996945	Rel. precision:	0.001000
Durbin-Watson Value:	0.183	t-critical(0.95;88):	1.978
Durbin-Watson Factor:	2.394		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.43	87	Cn B					
1	s:	1.14	1.43	88	Fn					
2	s:	1.29	1.43	88	C1 B					
3	s:	1.63	1.42	89	F2					
4	s:	1.70	1.42	89	B1					
5	s:	2.09	1.43	88	An					
6	s:	2.26	1.42	89	A3					
7	s:	2.49	1.42	89	A2					
8	s:	3.33	1.42	89	F1					
9	s:	8.45	1.42	89	R3					
10	s:	9.58	1.42	89	D1F					
11	s:	10.06	1.42	89	D3F					
12	s:	10.72	1.42	89	D3					
13	s:	13.52	1.42	89	R2					
14	s:	19.06	1.42	89	D4					
15	s:	25.36	1.42	89	D2					
16	s:	46.62	1.42	89	D1					

Sample 15 / cycle 4 / Fn
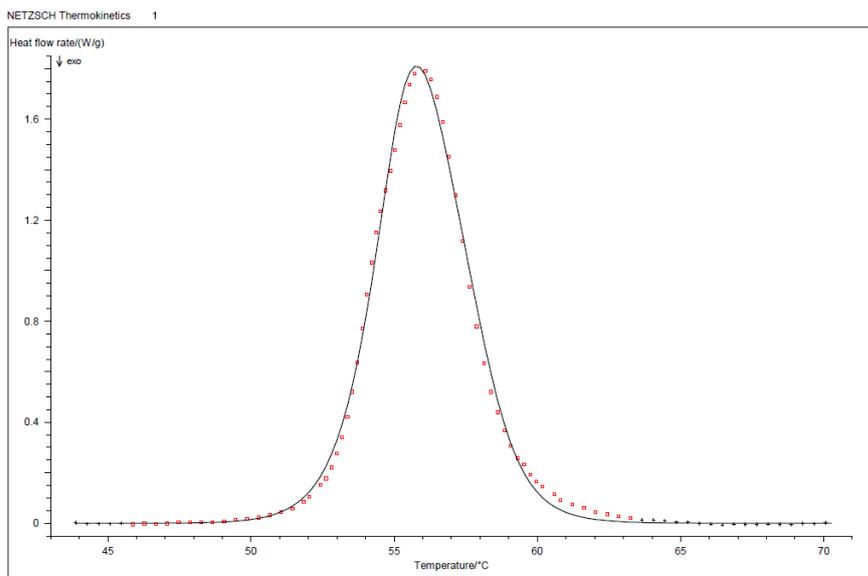
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 13:21

Project: 1
Model   1: n-th order with autocatalysis by B

$A \text{---} 1 \rightarrow B$

Start evaluation:	0.00050	Measurement type: DSC
Fine evaluation:	0.99950	
SCAN 1 Identity:		OP320 11.04.2016 14:04:20/Segm.S1/1
Transfer Corr:	204 F1.kcr	
Min. Temp/°C:	43.8720	Min. Time/min: 0.0
Max. Temp°C:	70.2618	Max. Time/min: 2.9519
Heating rate/(K/min):	8.940	Sampling time/s: 1.342
Sample mass/mg:	2.800	
Base line type:		LeftPts: 25 RightPts: 35

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	78.8448	145.4079				3.1815E-2
1	E1 kJ/mol	505.1724	921.4108			+	0.6604
2	React.ord. 1	1.5509	2.0786			+	0.2202
3	log Kcat 1	0.4500	-0.1854				0.2239
4	Area 1/(J/g)	50.9071	50.9071				constant

STATISTICS

Least squares:	4.36462	Number of cycles:	21
Mean of residues:	0.18115	Max.No of cycles:	50
Correlation coefficient:	0.998004	Rel. precision:	0.001000
Durbin-Watson Value:	0.180	t-critical(0.95;84):	1.980
Durbin-Watson Factor:	2.414		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.44	84	Cn B					
1	s:	1.11	1.43	86	F2					
2	s:	1.11	1.44	85	Fn					
3	s:	1.26	1.43	86	B1					
4	s:	1.28	1.44	85	C1 B					
5	s:	4.81	1.44	85	An					
6	s:	5.54	1.43	86	A3					
7	s:	6.16	1.43	86	A2					
8	s:	7.97	1.43	86	F1					
9	s:	17.08	1.43	86	R3					
10	s:	19.06	1.43	86	D1F					
11	s:	20.01	1.43	86	D3F					
12	s:	20.90	1.43	86	D3					
13	s:	25.08	1.43	86	R2					
14	s:	33.36	1.43	86	D4					
15	s:	46.52	1.43	86	D2					
16	s:	72.97	1.43	86	D1					

Sample 15 / cycle 5 / Fn

NETZSCH Thermokinetics   1

Heat flow rate/(W/g)
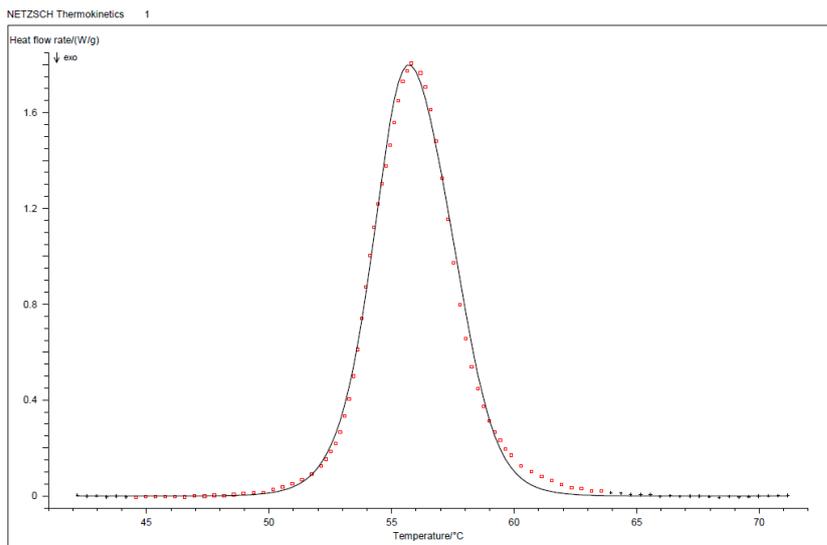
NETZSCH Thermokinetics
Date/Time: 30.11.2016 at 13:28

Project: 1
Model   1: n-th order

A—1→B

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP320 12.04.2016 10:38:01/Segm.S1/1		
Transfer Corr:	204_F1.kcr			
Min. Temp/°C:	42.1778	Min. Time/min:		0.0
Max. Temp/°C:	71.1674	Max. Time/min:		3.2448
Heating rate/(K/min):	8.934	Sampling time/s:		1.343
Sample mass/mg:	2.800			
Base line type:		LeftPts: 35		RightPts: 35

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	160.8132	157.6458				0.4489
1	E1 kJ/mol	1017.5484	997.6283			+	2.8708
2	React.ord. 1	2.1084	2.0226			+	8.3578E-2
3	Area 1/(J/g)	51.1202	51.1202				constant

STATISTICS

Least squares:	4.71062	Number of cycles:	7
Mean of residues:	0.17962	Max.No of cycles:	50
Correlation coefficient:	0.997750	Rel. precision:	0.001000
Durbin-Watson Value:	0.149	t-critical(0.95;95):	1.976
Durbin-Watson Factor:	2.644		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.41	94	Cn B					
1	s:	1.17	1.41	96	F2					
2	s:	1.18	1.41	95	Fn					
3	s:	1.21	1.41	96	B1					
4	s:	1.25	1.41	95	C1 B					
5	s:	5.16	1.41	95	An					
6	s:	5.59	1.41	96	A3					
7	s:	6.09	1.41	96	A2					
8	s:	7.84	1.41	96	F1					
9	s:	16.85	1.41	96	R3					
10	s:	18.68	1.41	96	D1F					
11	s:	19.74	1.41	96	D3F					
12	s:	20.73	1.41	96	D3					
13	s:	24.50	1.41	96	R2					
14	s:	33.53	1.41	96	D4					
15	s:	44.47	1.41	96	D2					
16	s:	73.77	1.41	96	D1					

Sample 15 / cycle 6 / Fn

NETZSCH Thermokinetics
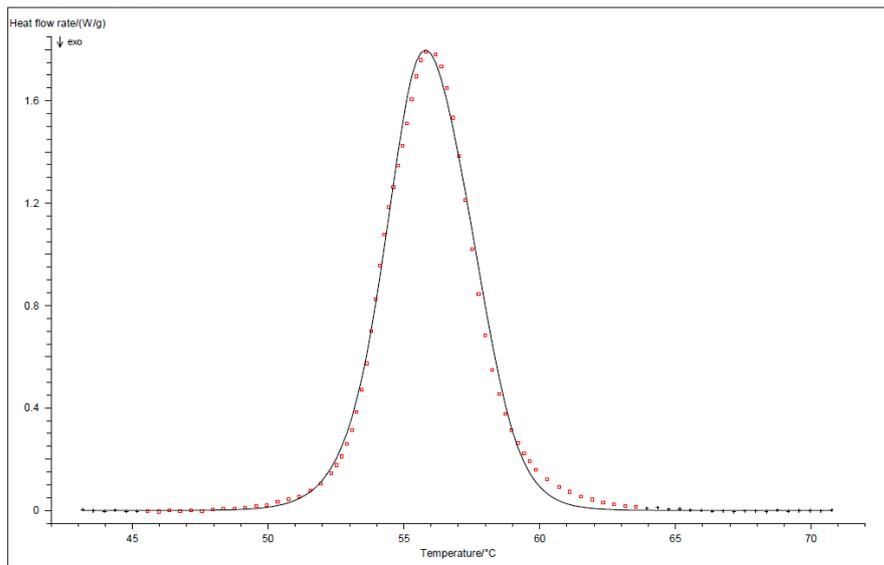
Date/Time: 30.11.2016 at 13:30

Project: 1
Model   1: n-th order

$A \longrightarrow 1 \rightarrow B$

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 12.04.2016 12:20:03/Segm.S1/3	
Transfer Corr:	204 F1.kcr		
Min. Temp/°C:	43.1695	Min. Time/min:	0.0
Max. Temp°C:	70.7586	Max. Time/min:	3.0876
Heating rate/(K/min):	8.936	Sampling time/s:	1.342
Sample mass/mg:	2.800		
Base line type:		LeftPts: 30	RightPts: 30

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	152.6114	152.6114				2.7285E-2
1	E1 kJ/mol	966.2781	966.2781			+	0.3799
2	React.ord. 1	1.9027	1.9027			+	0.1811
3	Area 1/(J/g)	50.6712	50.6712				constant

STATISTICS

Least squares:	4.86546	Number of cycles:	14
Mean of residues:	0.18709	Max.No of cycles:	50
Correlation coefficient:	0.997708	Rel. precision:	0.001000
Durbin-Watson Value:	0.156	t-critical(0.95;89):	1.978
Durbin-Watson Factor:	2.586		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.43	88	Cn B					
1	s:	1.16	1.42	89	Fn					
2	s:	1.18	1.42	90	F2					
3	s:	1.28	1.42	89	C1 B					
4	s:	1.33	1.42	90	B1					
5	s:	4.24	1.42	89	An					
6	s:	4.64	1.42	90	A3					
7	s:	5.13	1.42	90	A2					
8	s:	6.70	1.42	90	F1					
9	s:	15.12	1.42	90	R3					
10	s:	16.92	1.42	90	D1F					
11	s:	17.80	1.42	90	D3F					
12	s:	18.76	1.42	90	D3					
13	s:	22.13	1.42	90	R2					
14	s:	30.61	1.42	90	D4					
15	s:	42.19	1.42	90	D2					
16	s:	71.39	1.42	90	D1					

Sample 15 / cycle 7 / Fn
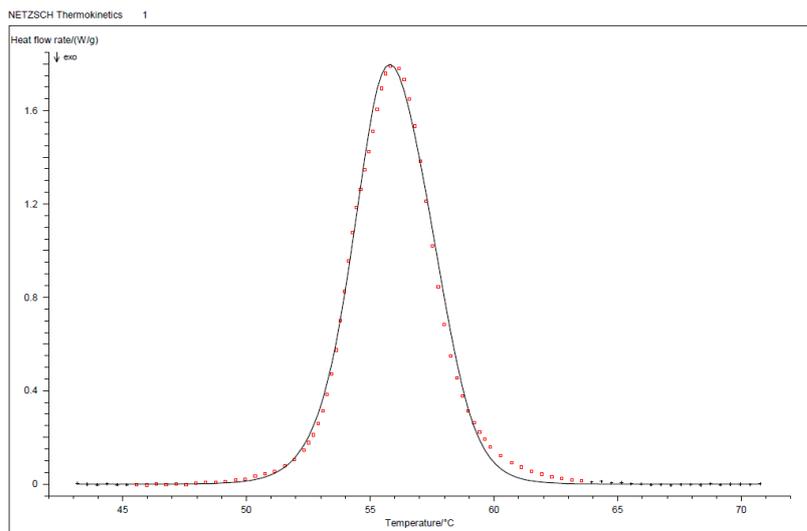
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 13:35

Project: 1
Model   1: n-th order

$A \longrightarrow 1 \rightarrow B$

Start evaluation:	0.00050
Fine evaluation:	0.99950
SCAN 1 Identity:	
Transfer Corr:	204 F1.kcr
Min. Temp/°C:	43.1695
Max. Temp°C:	70.7586
Heating rate/(K/min):	8.936
Sample mass/mg:	2.800
Base line type:	

Measurement type:	DSC
	OP320 12.04.2016 12:20:03/Segm.S1/3
Min. Time/min:	0.0
Max. Time/min:	3.0876
Sampling time/s:	1.342
LeftPts: 30	RightPts: 30

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	157.9722	152.6114				0.4996
1	E1 kJ/mol	999.9923	966.2781			+	3.1970
2	React.ord. 1	1.9940	1.9027			+	8.7621E-2
3	Area 1/(J/g)	50.6712	50.6712				constant

STATISTICS

Least squares:	4.86546	Number of cycles:	8
Mean of residues:	0.18709	Max.No of cycles:	50
Correlation coefficient:	0.997708	Rel. precision:	0.001000
Durbin-Watson Value:	0.156	t-critical(0.95;89):	1.978
Durbin-Watson Factor:	2.586		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2 Type 3 Type 4 Type 5 Type 6
0	s:	1.00	1.43	88	Cn B	
1	s:	1.16	1.42	89	Fn	
2	s:	1.18	1.42	90	F2	
3	s:	1.28	1.42	89	C1 B	
4	s:	1.33	1.42	90	B1	
5	s:	4.24	1.42	89	An	
6	s:	4.64	1.42	90	A3	
7	s:	5.13	1.42	90	A2	
8	s:	6.70	1.42	90	F1	
9	s:	15.12	1.42	90	R3	
10	s:	16.92	1.42	90	D1F	
11	s:	17.80	1.42	90	D3F	
12	s:	18.76	1.42	90	D3	
13	s:	22.13	1.42	90	R2	
14	s:	30.61	1.42	90	D4	
15	s:	42.19	1.42	90	D2	
16	s:	71.39	1.42	90	D1	

Sample 18 / cycle 2 / Fn

NETZSCH Thermokinetics

NETZSCH Thermokinetics
Project: 1
Model   1: n-th order

Date/Time: 30.11.2016 at 16:06

A—1→B

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP320 27.05.2016 11:00:44/Segm.S1/3		
Transfer Corr:	204 F1.kcr			
Min. Temp/°C:	35.5835	Min. Time/min:		0.0
Max. Temp°C:	56.1072	Max. Time/min:		2.2997
Heating rate/(K/min):	8.925	Sampling time/s:		0.336
Sample mass/mg:	3.360			
Base line type:		LeftPts: 9	RightPts: 10	

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	318.9720	318.9720				1.1533E-2
1	E1 kJ/mol	1948.4247	1948.4247			+	0.1394
2	React.ord. 1	1.9923	1.9923			+	6.1883E-2
3	Area 1/(J/g)	52.0084	52.0084				constant

STATISTICS

Least squares:	14.78676	Number of cycles:	12
Mean of residues:	0.18945	Max.No of cycles:	50
Correlation coefficient:	0.996398	Rel. precision:	0.001000
Durbin-Watson Value:	0.014	t-critical(0.95;183):	1.964
Durbin-Watson Factor:	8.503		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.28	182	Cn B					
1	s:	2.89	1.28	183	C1 B					
2	s:	3.58	1.28	184	F2					
3	s:	3.60	1.28	183	Fn					
4	s:	4.29	1.28	184	B1					
5	s:	5.07	1.28	183	An					
6	s:	5.41	1.28	184	A3					
7	s:	7.26	1.28	184	A2					
8	s:	17.35	1.28	184	F1					
9	s:	36.63	1.28	184	R3					
10	s:	46.87	1.28	184	D1F					
11	s:	52.48	1.28	184	R2					
12	s:	56.72	1.28	184	D3F					
13	s:	62.29	1.28	184	D3					
14	s:	96.77	1.28	184	D4					
15	s:	116.97	1.28	184	D2					
16	s:	174.48	1.28	184	D1					
17	s:	439.66	1.26	223	Bna					

Sample 18 / cycle 3 / Fn

NETZSCH Thermokinetics   1
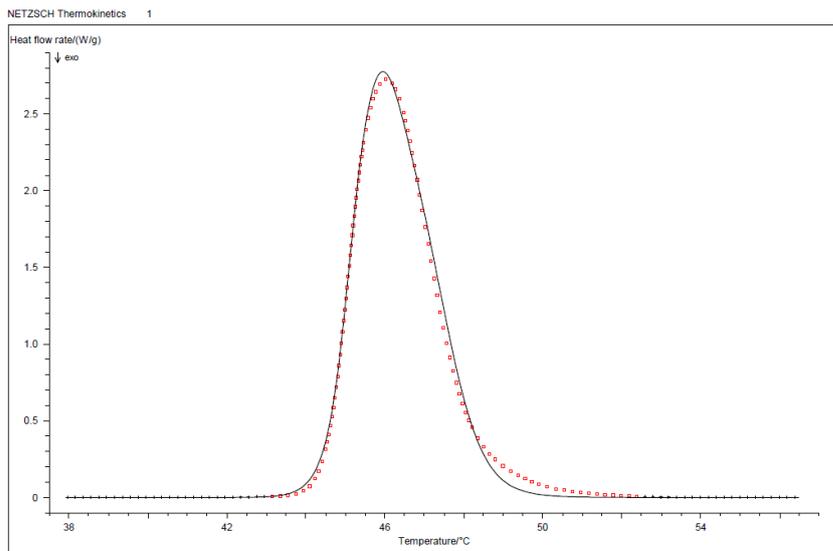
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 16:08

Project: 1
Model   1: n-th order

A—1→B

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP320 30.05.2016 11:22:18/Segm.S1/3		
Transfer Corr:	204_F1.kcr			
Min. Temp/°C:	37.9569	Min. Time/min:		0.0
Max. Temp/°C:	56.4834	Max. Time/min:		2.0795
Heating rate/(K/min):	8.909	Sampling time/s:		0.336
Sample mass/mg:	3.360			
Base line type:		LeftPts: 25		RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	367.2922	397.8562				1.4225E-2
1	E1 kJ/mol	2246.3037	2432.4769			+	0.1101
2	React.ord. 1	2.6415	2.7863			+	4.3993E-2
3	Area 1/(J/g)	52.9368	52.9368				constant

STATISTICS

Least squares:	6.59243	Number of cycles:	21
Mean of residues:	0.13312	Max.No of cycles:	50
Correlation coefficient:	0.998617	Rel. precision:	0.001000
Durbin-Watson Value:	0.018	t-critical(0.95;185):	1.964
Durbin-Watson Factor:	7.511		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.28	185	Fn					
1	s:	2.90	1.28	186	F2					
2	s:	4.00	1.28	184	Cn B					
3	s:	5.70	1.28	185	C1 B					
4	s:	5.73	1.28	186	B1					
5	s:	8.08	1.28	185	An					
6	s:	8.39	1.28	186	A3					
7	s:	10.02	1.28	186	A2					
8	s:	19.45	1.28	186	F1					
9	s:	35.39	1.28	186	R3					
10	s:	47.46	1.28	186	D1F					
11	s:	47.48	1.28	186	R2					
12	s:	54.49	1.28	186	D3F					
13	s:	57.79	1.28	186	D3					
14	s:	81.27	1.28	186	D4					
15	s:	99.02	1.28	186	D2					
16	s:	134.42	1.28	186	D1					
17	s:	276.93	1.26	223	Bna					

Sample 19 / cycle 1 / Fn
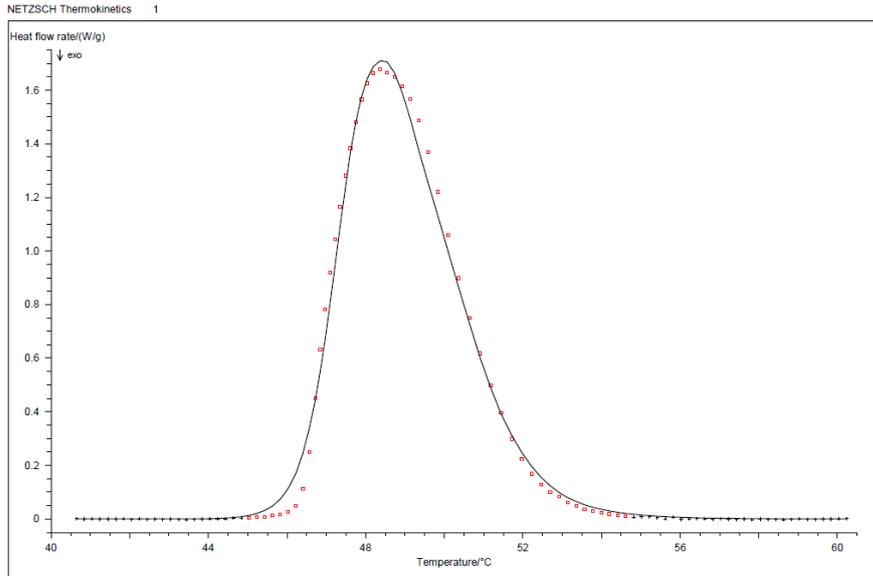
NETZSCH Thermokinetics

Date/Time: 30.11.2016 at 13:37

Project: 1
Model   1: n-th order

A —1→ B

Start evaluation:	0.00050	Measurement type:		DSC
Fine evaluation:	0.99950			
SCAN 1 Identity:		OP320 14.04.2016 13:48:15/Segm.S1/3		
Transfer Corr:	204_F1.kcr			
Min. Temp/°C:	40.6485	Min. Time/min:		0.0
Max. Temp°C:	60.2333	Max. Time/min:		2.1924
Heating rate/(K/min):	8.933	Sampling time/s:		1.342
Sample mass/mg:	4.660			
Base line type:		LeftPts: 25		RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	194.2286	296.5000				3.7808E-2
1	E1 kJ/mol	1200.2375	1827.4645			+	0.5466
2	React.ord. 1	2.3132	3.5589			+	0.3272
3	Area 1/(J/g)	43.2735	43.2735				constant

STATISTICS

Least squares:	7.56068	Number of cycles:	20
Mean of residues:	0.27635	Max.No of cycles:	50
Correlation coefficient:	0.995983	Rel. precision:	0.001000
Durbin-Watson Value:	0.212	t-critical(0.95;46):	2.004
Durbin-Watson Factor:	2.232		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.64	46	Fn					
1	s:	1.51	1.64	45	Cn B					
2	s:	3.12	1.64	46	C1 B					
3	s:	3.37	1.63	47	B1					
4	s:	3.38	1.63	47	F2					
5	s:	4.82	1.64	46	An					
6	s:	8.20	1.63	47	A2					
7	s:	12.72	1.63	47	F1					
8	s:	20.46	1.63	47	R3					
9	s:	24.77	1.63	47	D1F					
10	s:	25.77	1.63	47	R2					
11	s:	26.31	1.63	47	A3					
12	s:	27.13	1.63	47	D3F					
13	s:	27.94	1.63	47	D3					
14	s:	37.04	1.63	47	D4					
15	s:	43.33	1.63	47	D2					
16	s:	59.79	1.63	47	D1					

Sample 19 / cycle 2 / Fn

NETZSCH Thermokinetics   Date/Time: 30.11.2016 at 13:40
Project: 1
Model   1: n-th order   A — 1 → B

Start evaluation: 0.00050   Measurement type: DSC
Fine evaluation: 0.99950
SCAN 1   Identity: OP320 14.04.2016 15:04:45/Segm.S1/3
Transfer Corr: 204_F1.kcr
Min. Temp/°C: 36.3948   Min. Time/min: 0.0
Max. Temp/°C: 57.7620   Max. Time/min: 2.3946
Heating rate/(K/min):   8.923   Sampling time/s: 1.343
Sample mass/mg: 4.660
Base line type: LeftPts: 25   RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	476.8918	322.1788				0.1323
1	E1 kJ/mol	2912.3566	1970.4791			+	0.8821
2	React.ord. 1	4.4001	2.8594			+	0.1316
3	Area 1/(J/g)	46.6758	46.6758				constant

STATISTICS
Least squares: 6.48893   Number of cycles: 11
Mean of residues: 0.24512   Max.No of cycles: 50
Correlation coefficient: 0.997200 Rel. precision: 0.001000
Durbin-Watson Value: 0.965   t-critical(0.95;42):   2.009
Durbin-Watson Factor: 1.169

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.69	41	Cn B					
1	s:	1.02	1.68	42	Fn					
2	s:	2.31	1.67	43	F2					
3	s:	2.65	1.68	42	C1 B					
4	s:	2.81	1.67	43	B1					
5	s:	4.25	1.68	42	An					
6	s:	5.91	1.67	43	A2					
7	s:	12.21	1.67	43	F1					
8	s:	21.41	1.67	43	R3					
9	s:	28.30	1.67	43	R2					
10	s:	29.01	1.67	43	D1F					
11	s:	34.16	1.67	43	D3F					
12	s:	35.66	1.67	43	D3					
13	s:	50.56	1.67	43	D4					
14	s:	55.25	1.67	43	D2					
15	s:	79.88	1.67	43	D1					
16	s:	362.45	1.67	43	A3					

Sample 19 / cycle 3 / Fn
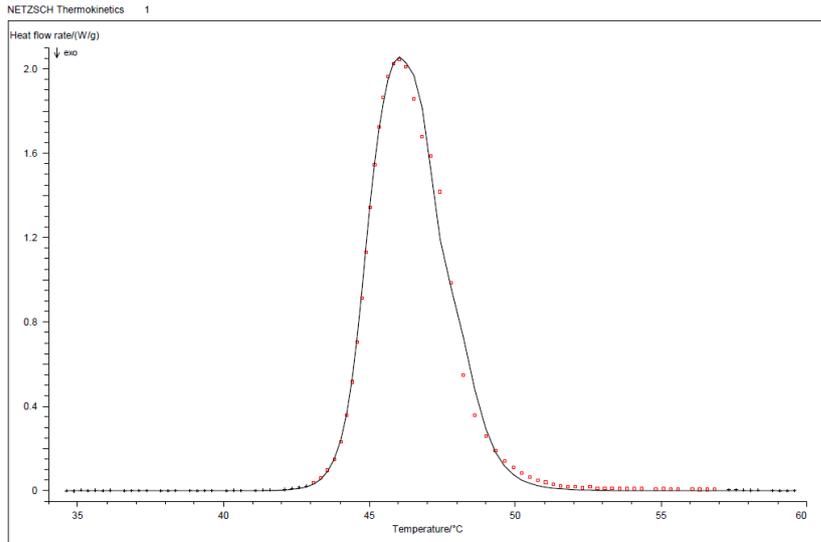
NETZSCH Thermokinetics

Project: 1
Model 1: n-th order

Date/Time: 30.11.2016 at 13:42

A—1→B

Start evaluation:	0.00050	Measurement type:	DSC
Fine evaluation:	0.99950		
SCAN 1 Identity:		OP320 14.04.2016 16:11:03/Segm.S1/3
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	34.6119	Min. Time/min:	0.0
Max. Temp°C:	59.5753	Max. Time/min:	2.7964
Heating rate/(K/min):	8.927	Sampling time/s:	1.678
Sample mass/mg:	4.660		
Base line type:		LeftPts: 25	RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sign	t*Std.Dev.
0	log A1/s^-1	483.7347	303.1342				3.1344E-2
1	E1 kJ/mol	2953.7593	1854.4685			+	0.6480
2	React.ord. 1	4.8918	2.8607			+	0.3543
3	Area 1/(J/g)	47.7439	47.7439				constant

STATISTICS

Least squares:	7.14956	Number of cycles:	23
Mean of residues:	0.26606	Max.No of cycles:	50
Correlation coefficient:	0.997324	Rel. precision:	0.001000
Durbin-Watson Value:	1.149	t-critical(0.95;54):	1.996
Durbin-Watson Factor:	1.105		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-act	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.57	54	Fn					
1	s:	1.02	1.58	53	Cn B					
2	s:	1.93	1.57	55	F2					
3	s:	2.12	1.57	54	C1 B					
4	s:	2.20	1.57	55	B1					
5	s:	3.55	1.57	54	An					
6	s:	4.56	1.57	55	A2					
7	s:	8.97	1.57	55	F1					
8	s:	15.54	1.57	55	R3					
9	s:	19.70	1.57	55	R2					
10	s:	20.82	1.57	55	D1F					
11	s:	24.38	1.57	55	D3F					
12	s:	25.01	1.57	55	D3					
13	s:	33.65	1.57	55	D4					
14	s:	39.05	1.57	55	D2					
15	s:	59.90	1.57	55	D1					
16	s:	90.10	1.57	55	A3					