Electronic Supplementary Information

Compensation effects and relation between the activation energy of spin transition and the hysteresis loop width for an iron(II) complex

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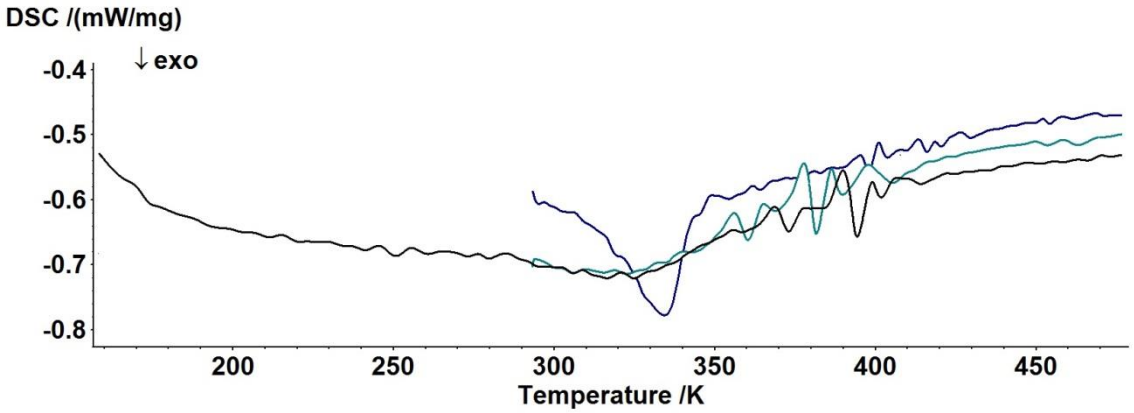


Fig. S1 Typical DSC curves for the $\mathbf{1}^{A/HS} \rightarrow \mathbf{1}^{A/LS}$ transition (cycle 6 (blue), cycle 29 (green) and cycle 31 (black).

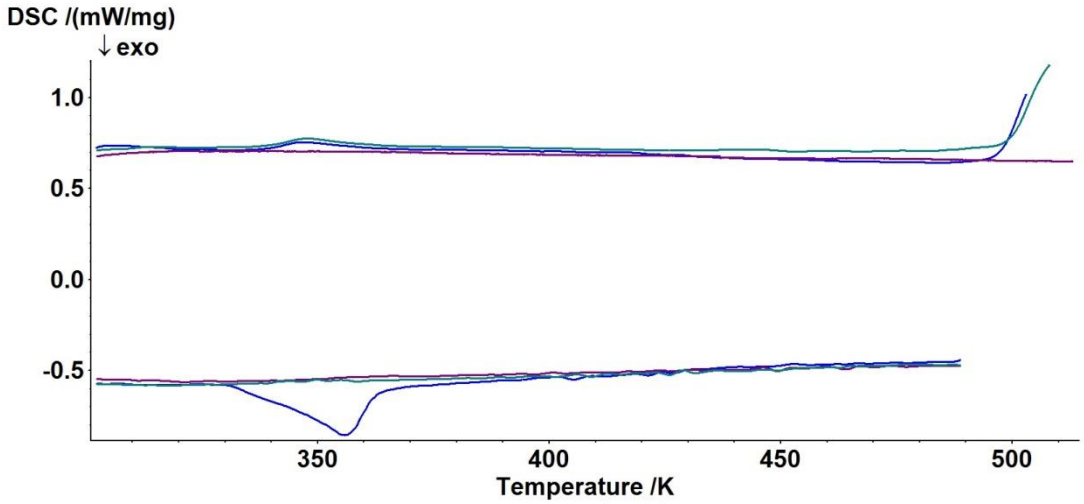


Fig. S2 DSC curves for the $\mathbf{1}^{A/LS} \rightarrow \mathbf{1}^{A/HS}$ and $\mathbf{1}^{A/HS} \rightarrow \mathbf{1}^{A/LS}$ transitions, a separate sample, cycle 5 (blue, 300 – 500 – 300 K), cycle 6 (green, 300 – 505 – 300 K) and cycle 7 (violet, 300 – 510 – 300 K).

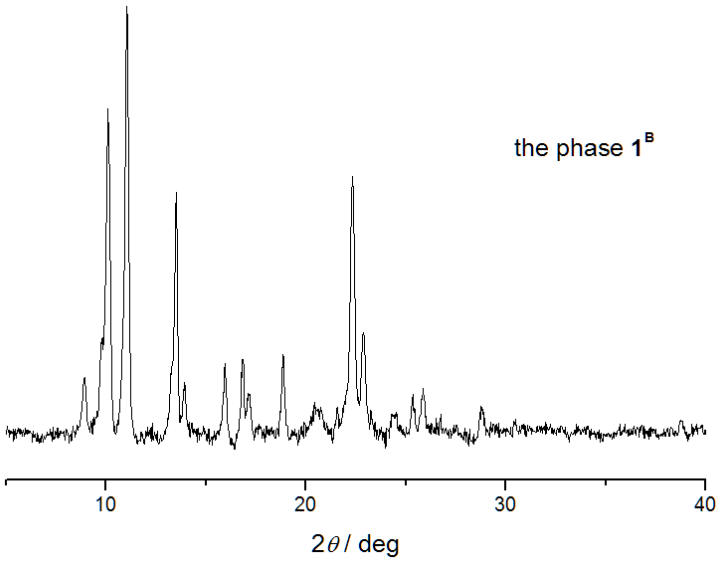


Fig. S3 X-ray powder pattern of the product (the phase $\mathbf{1}^{B}$) after cycle 7 (see Fig. S2).

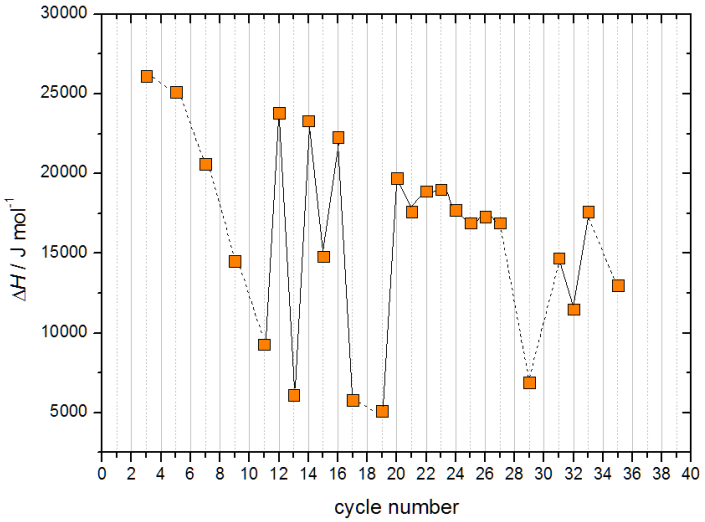


Fig. S4 Evolution of the enthalpy of the $\mathbf{1}^{\mathbf{A/LS}} \rightarrow \mathbf{1}^{\mathbf{A/HS}}$ transition on multiple cycling.

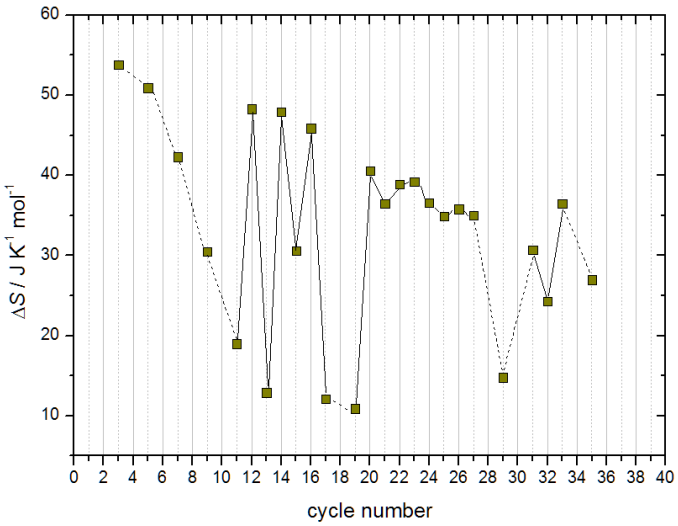


Fig. S5 Evolution of the entropy of the $\mathbf{1}^{\mathbf{A/LS}} \rightarrow \mathbf{1}^{\mathbf{A/HS}}$ transition on multiple cycling.

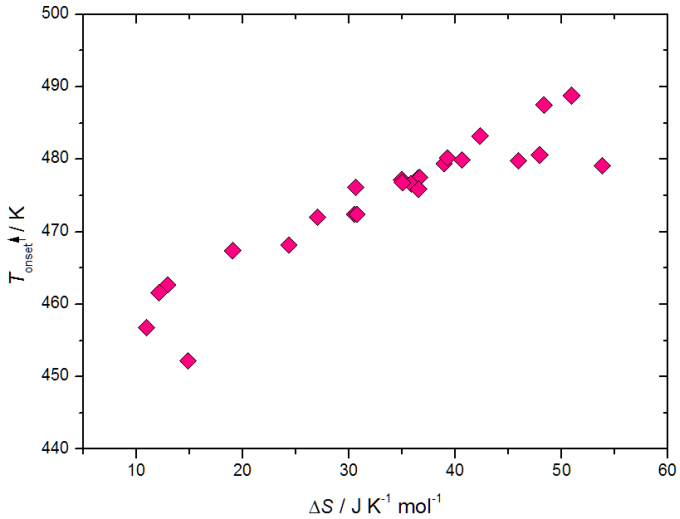


Fig. S6 Correlation between the $T_{onset}\uparrow$ and the entropy of the $\mathbf{1}^{\mathbf{A/LS}} \rightarrow \mathbf{1}^{\mathbf{A/HS}}$ spin transition.

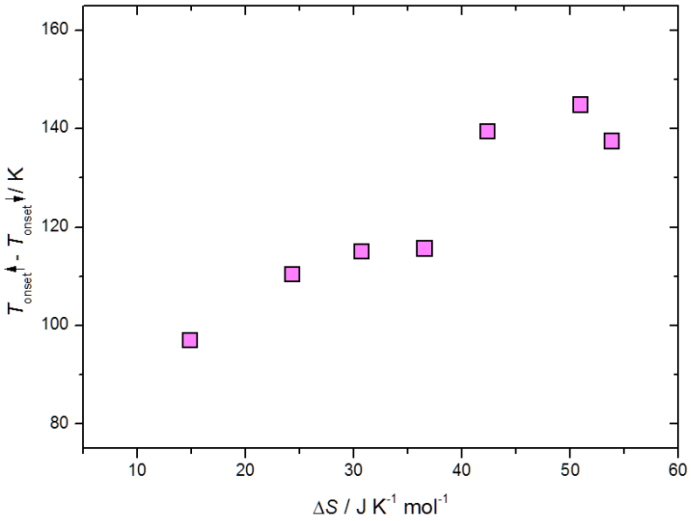


Fig. S7 Correlation between the hysteresis loop width and the entropy of the $\mathbf{1}^{\mathbf{A/LS}} \rightarrow \mathbf{1}^{\mathbf{A/HS}}$ transition.

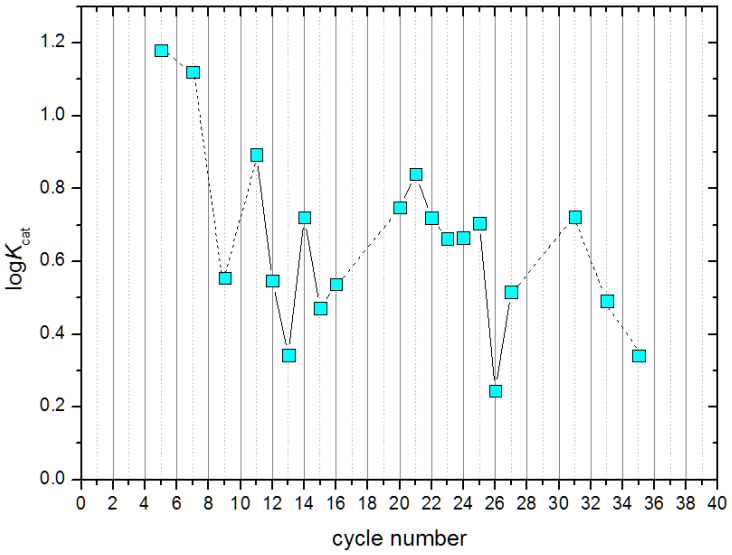


Fig. S8 Evolution of the logK_{cat} for the $\mathbf{1}^{A/LS} \rightarrow \mathbf{1}^{A/HS}$ transition on multiple cycling (the CnB model).

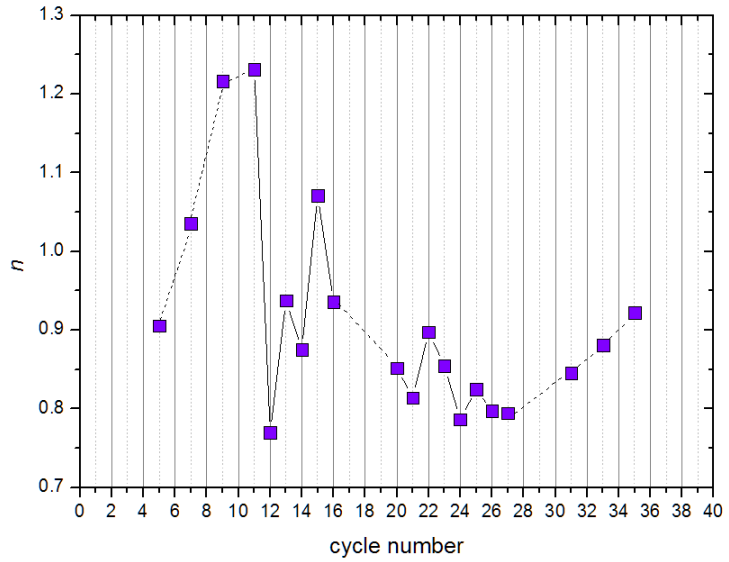


Fig. S9 Evolution of the reaction order, *n*, for the $\mathbf{1}^{A/LS} \rightarrow \mathbf{1}^{A/HS}$ transition on multiple cycling (the CnB model).

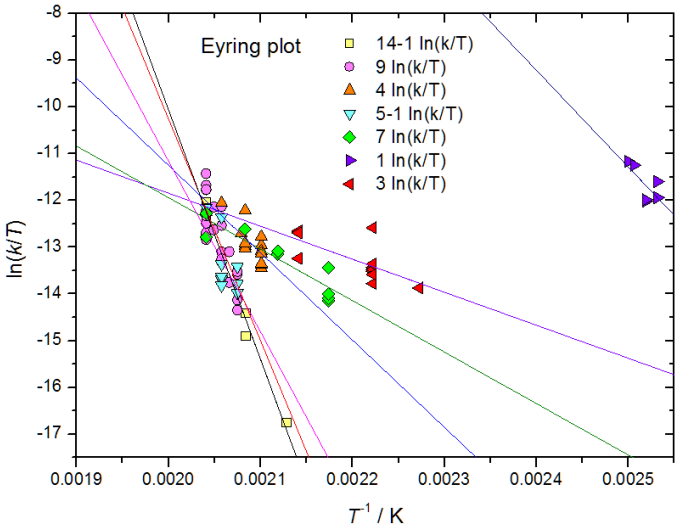


Fig. S10 The Eyring plot for the samples **14-1**, **9**, **4**, **5-1**, **7**, **3** and **1**.

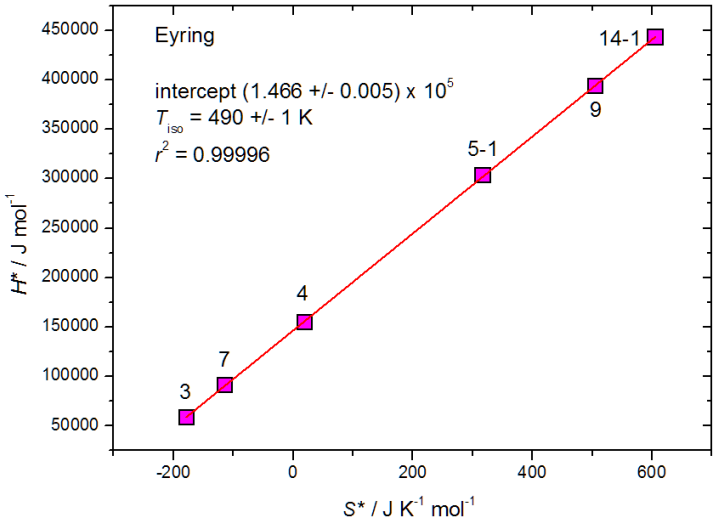


Fig. S11 The enthalpy-entropy compensation for the *H** and *S** values derived from the Eyring plot (see Fig. S10, samples **14-1**, **9**, **4**, **5-1**, **7** and **3**).

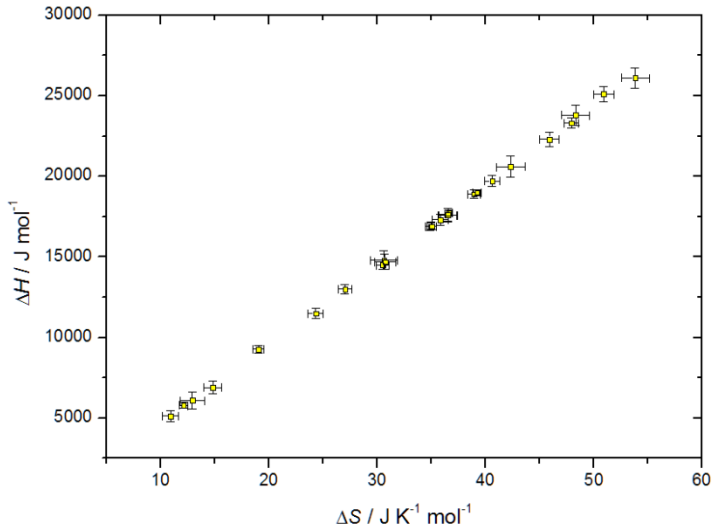


Fig. S12 The enthalpy-entropy compensation for the $\mathbf{1}^{\mathbf{A/LS}} \rightarrow \mathbf{1}^{\mathbf{A/HS}}$ spin transition, error bars are shown.

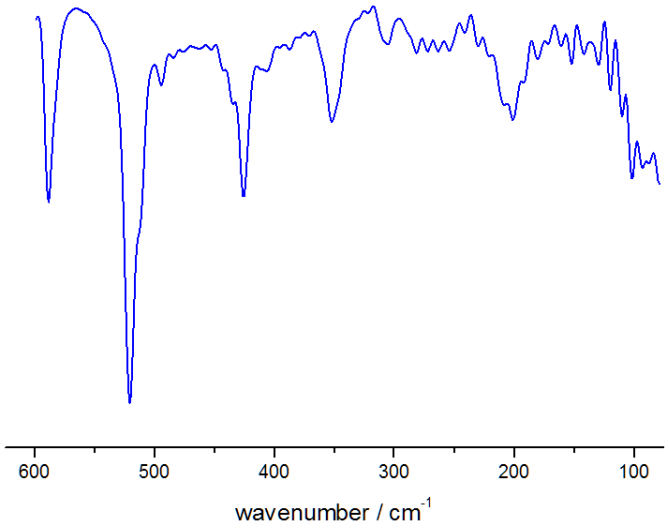


Fig. S13 Far IR spectrum of the phase $\mathbf{1}^{A/LS}$.

Cycle 5 / Activation energy

NETZSCH Thermokinetics

Date/Time: 04.02.2016 at 13:37

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 255 17.01.2014 12:57:52/Segm.S1/3	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	87.7867	Min. Time/min:	0.0
Max. Temp°C:	227.7923	Max. Time/min:	23.3274
Heating rate/(K/min):	6.002	Sampling time/s:	4.999
Sample mass/mg:	1.330		
Base line type:		LeftPts: 20	RightPts: 20

PARAMETERS AND STANDARD DEVIATIONS

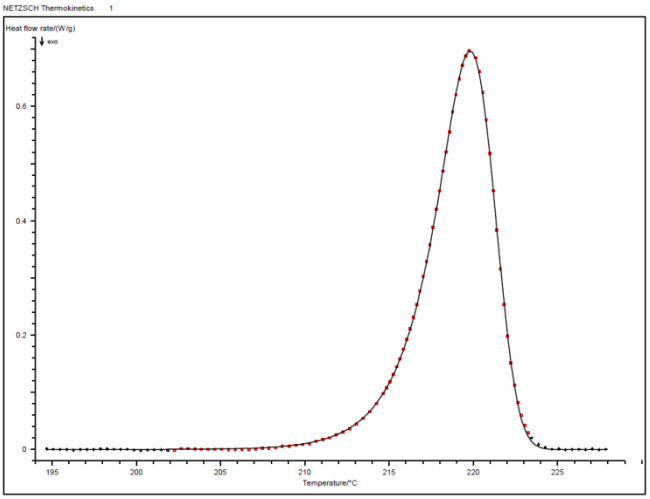
#	Parameter	Initial Val.	Optimum Val.	Minimun	Maximun	Sigrt*Std.Dev.
0	log A1/s^-1	153.3196	42.8985			0.1528
1	E1 kJ/mol	1456.3173	427.1194			+ 1.5151
2	React.ord. 1	2.7567	0.9055			6.2426E-2
3	log Kcat 1	0.4500	1.1801			2.5865E-2
4	Area 1/(J/g)	37.0966	37.0966			constant

STATISTICS

Least squares:	0.11935	Number of cycles:	9
Mean of residues:	2.06094E-2	Max.No of cycles:	50
Correlation coefficient:	0.998770	Rel. precision:	0.001000
Durbin-Watson Value:	0.084	t-critical(0.95;260):	1.960
Durbin-Watson Factor:	3.493		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-ac	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.23	260	Cn B					
1	s:	1.16	1.23	261	C1 B					
2	s:	1.90	1.26	176	Bna					
3	s:	3.19	1.23	262	A3					
4	s:	3.46	1.23	262	A2					



Cycle 7 / Activation energy

NETZSCH Thermokinetics

Date/Time: 04.02.2016 at 16:11

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 255 20.01.2014 12:50:45/Segm.S1/3	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	188.9538	Min. Time/min:	0.0
Max. Temp°C:	227.7564	Max. Time/min:	6.4660
Heating rate/(K/min):	6.001	Sampling time/s:	2.000
Sample mass/mg:	1.330		
Base line type:		LeftPts: 6	RightPts: 6

PARAMETERS AND STANDARD DEVIATIONS

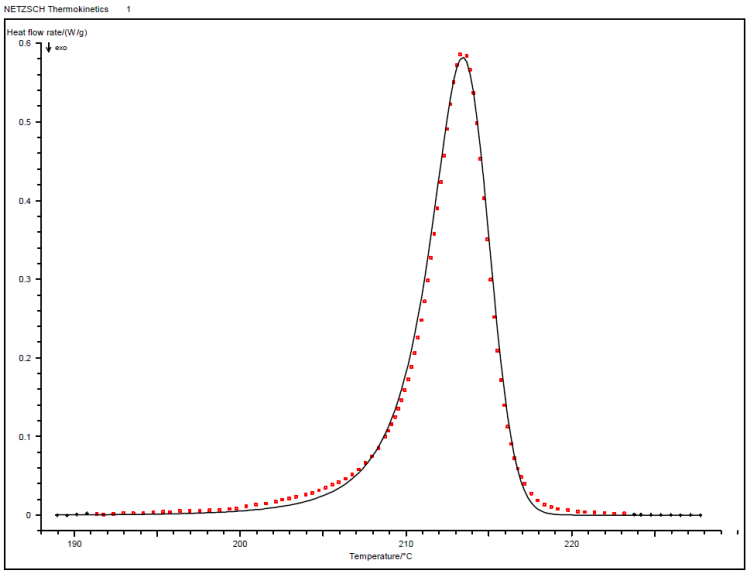
#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sigrt*Std.Dev.
0	log A1/s^-1	117.1282	52.5584			7.6833E-3
1	E1 kJ/mol	1105.2497	510.3558			+ 0.1559
2	React.ord. 1	1.5070	1.0359			8.2401E-2
3	log Kcat 1	0.4500	1.1204			1.0646E-2
4	Area 1/(J/g)	29.2507	29.2507			constant

STATISTICS

Least squares:	0.43749	Number of cycles:	18
Mean of residues:	4.73659E-2	Max.No of cycles:	50
Correlation coefficient:	0.997672	Rel. precision:	0.001000
Durbin-Watson Value:	0.037	t-critical(0.95;156):	1.966
Durbin-Watson Factor:	5.254		

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	156	Cn B					
1	s:	1.01	1.30	157	C1 B					
2	s:	3.13	1.30	157	An					
3	s:	3.45	1.30	158	A3					
4	s:	3.45	1.30	158	D1F					



Cycle 9 / Activation energy

NETZSCH Thermokinetics

Date/Time: 03.02.2016 at 11:55

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 255 09.07.2015 12:21:12/Segm.S1/1	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	172.8490	Min. Time/min:	0.0
Max. Temp°C:	227.6548	Max. Time/min:	9.1313
Heating rate/(K/min):	6.002	Sampling time/s:	2.000
Sample mass/mg:	1.310		
Base line type:	tangent area prop.	LeftPts: 60	RightPts: 10

PARAMETERS AND STANDARD DEVIATIONS

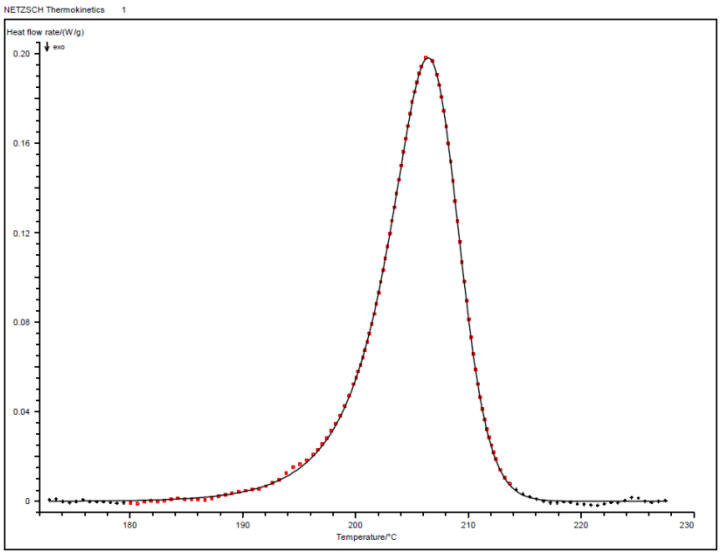
#	Parameter	Initial Val.	Optimum Val.	Minimun	Maximum	Sigrt*Std.Dev.
0	log A1/s^-1	51.6221	45.1316			4.7623E-3
1	E1 kJ/mol	490.9298	432.2438			+ 0.1080
2	React.ord. 1	1.3277	1.2163			3.0724E-2
3	log Kcat 1	0.4500	0.5550			5.5587E-3
4	Area 1/(J/g)	17.0678	17.0678			constant

STATISTICS

Least squares:	1.51363E-3	Number of cycles:	23
Mean of residues:	2.34609E-3	Max.No of cycles:	50
Correlation coefficient:	0.999935	Rel. precision:	0.001000
Durbin-Watson Value:	0.048	t-critical(0.95;166):	1.965
Durbin-Watson Factor:	4.614		

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	166	Cn B					
1	s:	3.55	1.29	167	C1 B					
2	s:	25.93	1.29	167	Fn					
3	s:	36.89	1.29	168	A3					
4	s:	37.12	1.29	167	An					



Cycle 11 / Activation energy

NETZSCH Thermokinetics

Date/Time: 03.02.2016 at 12:00

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 255 13.07.2015 13:43:30/Segm.S1/1	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	168.5396	Min. Time/min:	0.0
Max. Temp°C:	227.5444	Max. Time/min:	9.8324
Heating rate/(K/min):	6.001	Sampling time/s:	2.000
Sample mass/mg:	1.310		
Base line type:	tangent area prop.	LeftPts: 60	RightPts: 20

PARAMETERS AND STANDARD DEVIATIONS

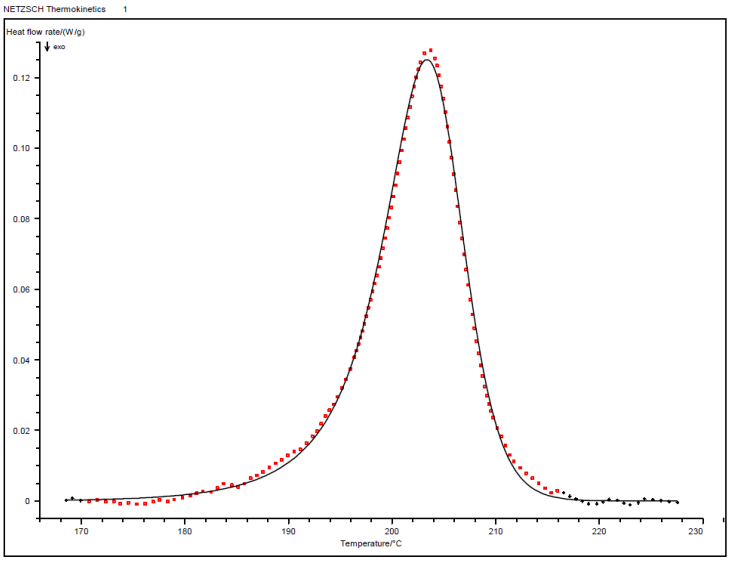
#	Parameter	Initial Val.	Optimum Val.	Minimun	Maximun	Sigrt*	Std.Dev.
0	log A1/s^-1	46.6215	28.5438				1.3695E-2
1	E1 kJ/mol	442.6073	281.4441			+	0.2261
2	React.ord. 1	1.4984	1.2315				2.9955E-2
3	log Kcat 1	0.4500	0.8939				2.4717E-2
4	Area 1/(J/g)	13.5750	13.5750				constant

STATISTICS

Least squares:	1.08352E-2	Number of cycles:	20
Mean of residues:	6.05026E-3	Max.No of cycles:	50
Correlation coefficient:	0.999007	Rel. precision:	0.001000
Durbin-Watson Value:	0.022	t-critical(0.95;225):	1.962
Durbin-Watson Factor:	6.830		

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	225	Cn B					
1	s:	1.69	1.25	226	C1 B					
2	s:	5.19	1.25	226	Fn					
3	s:	6.68	1.25	227	A2					
4	s:	6.68	1.25	227	F1					



Cycle 12 / Activation energy

NETZSCH Thermokinetics

Date/Time: 03.02.2016 at 12:02

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 255 15.07.2015 14:30:24/Segm.S1/1	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	186.0045	Min. Time/min:	0.0
Max. Temp°C:	227.6129	Max. Time/min:	6.9313
Heating rate/(K/min):	6.003	Sampling time/s:	1.999
Sample mass/mg:	1.310		
Base line type:	tangent area prop.	LeftPts: 69	RightPts: 6

PARAMETERS AND STANDARD DEVIATIONS

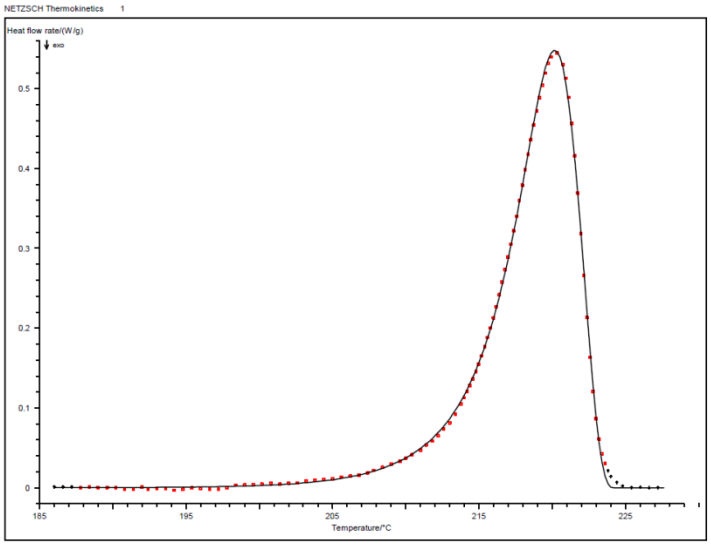
#	Parameter	Initial Val.	Optimum Val.	Minimun	Maximun	Sigrt*	Std.Dev.
0	log A1/s^-1	48.0627	48.8243				9.6161E-2
1	E1 kJ/mol	471.9764	479.4456			+	0.9026
2	React.ord. 1	0.7396	0.7703				4.5366E-2
3	log Kcat 1	0.4500	0.5474				2.2765E-2
4	Area 1/(J/g)	34.4846	34.4846				constant

STATISTICS

Least squares:	4.03317E-2	Number of cycles:	23
Mean of residues:	1.38915E-2	Max.No of cycles:	50
Correlation coefficient:	0.999801	Rel. precision:	0.001000
Durbin-Watson Value:	0.169	t-critical(0.95;176):	1.965
Durbin-Watson Factor:	2.483		

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	176	Cn B					
1	s:	2.95	1.28	178	D1F					
2	s:	3.84	1.28	178	D3F					
3	s:	8.73	1.28	177	Fn					
4	s:	9.50	1.28	178	R3					



Cycle 13 / Activation energy

NETZSCH Thermokinetics

Date/Time: 03.02.2016 at 12:08

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 255 15.07.2015 15:15:05/Segm.S1/1	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	164.1847	Min. Time/min:	0.0
Max. Temp°C:	221.3876	Max. Time/min:	19.0684
Heating rate/(K/min):	3.000	Sampling time/s:	4.000
Sample mass/mg:	1.310		
Base line type:	tangent area prop.	LeftPts: 45	RightPts: 25

PARAMETERS AND STANDARD DEVIATIONS

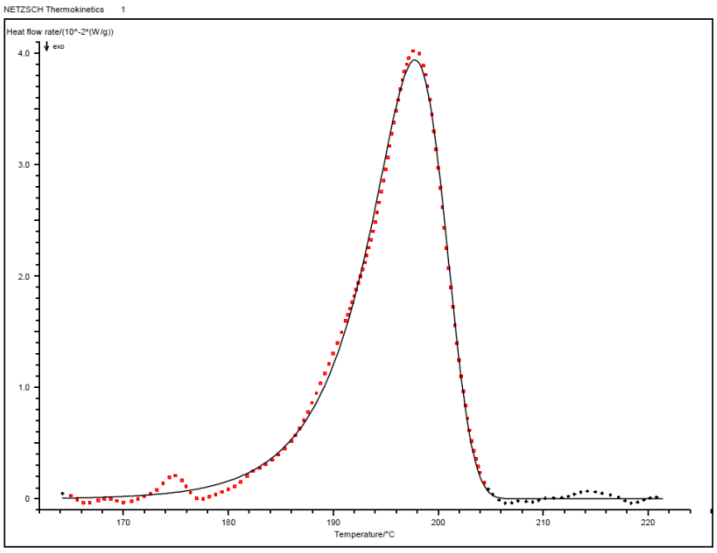
#	Parameter	Initial Val.	Optimum Val.	Minimun	Maximun	Sigrt*Std.Dev.
0	log A1/s^-1	33.6667	34.7055			3.8540E-2
1	E1 kJ/mol	324.5504	333.2500			+ 0.6258
2	React.ord. 1	0.9607	0.9379			+ 0.1936
3	log Kcat 1	0.4500	0.3421			3.5439E-2
4	Area 1/(J/g)	7.9615	7.9615			constant

STATISTICS

Least squares:	1.42699E-3	Number of cycles:	23
Mean of residues:	2.22982E-3	Max.No of cycles:	50
Correlation coefficient:	0.998643	Rel. precision:	0.001000
Durbin-Watson Value:	0.026	t-critical(0.95;195):	1.963
Durbin-Watson Factor:	6.249		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-ac	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.27	195	Cn B					
1	s:	1.12	1.27	196	C1 B					
2	s:	2.11	1.27	196	Fn					
3	s:	2.53	1.27	197	D1F					
4	s:	2.71	1.27	197	F1					



Cycle 14 / Activation energy

NETZSCH Thermokinetics

Date/Time: 03.02.2016 at 12:14

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 255 16.07.2015 11:58:57/Segm.S1/1	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	178.2721	Min. Time/min:	0.0
Max. Temp°C:	227.4767	Max. Time/min:	8.1988
Heating rate/(K/min):	6.001	Sampling time/s:	2.000
Sample mass/mg:	1.310		
Base line type:	tangent area prop.	LeftPts: 60	RightPts: 20

PARAMETERS AND STANDARD DEVIATIONS

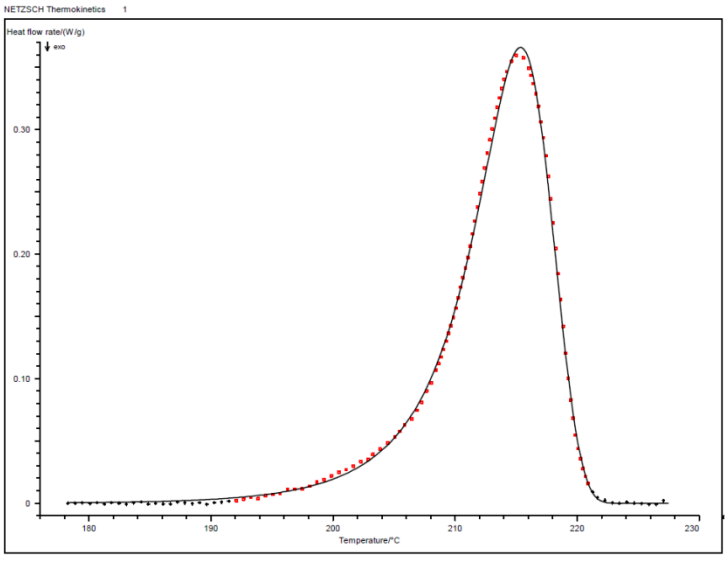
#	Parameter	Initial Val.	Optimum Val.	Minimun	Maximun	Sigrt*Std.Dev.
0	log A1/s^-1	41.8559	31.4675			1.2385E-2
1	E1 kJ/mol	409.6643	314.8270			+ 0.2317
2	React.ord. 1	1.0311	0.8754			8.2860E-2
3	log Kcat 1	0.4500	0.7214			1.2664E-2
4	Area 1/(J/g)	33.1670	33.1670			constant

STATISTICS

Least squares:	4.26554E-2	Number of cycles:	20
Mean of residues:	1.31413E-2	Max.No of cycles:	50
Correlation coefficient:	0.999470	Rel. precision:	0.001000
Durbin-Watson Value:	0.066	t-critical(0.95;142):	1.968
Durbin-Watson Factor:	3.915		

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	142	Cn B					
1	s:	1.95	1.32	143	C1 B					
2	s:	4.07	1.32	143	Fn					
3	s:	4.10	1.32	142	Bna					
4	s:	6.10	1.32	144	A3					



Cycle 15 / Activation energy

NETZSCH Thermokinetics

Date/Time: 03.02.2016 at 12:52

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:		Op 255 16.07.2015 15:15:29/Segm.S1/1	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	176.5422	Min. Time/min:	0.0
Max. Temp°C:	227.3505	Max. Time/min:	4.2318
Heating rate/(K/min):	12.006	Sampling time/s:	1.000
Sample mass/mg:	1.310		
Base line type:	tangent area prop.	LeftPts: 50	RightPts: 15

PARAMETERS AND STANDARD DEVIATIONS

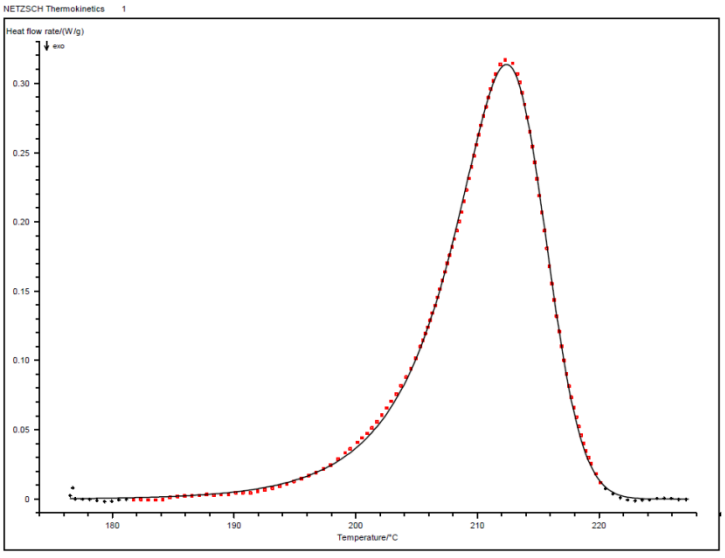
#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sigrt*Std.Dev.
0	log A1/s^-1	36.8853	35.5669			1.2441E-2
1	E1 kJ/mol	358.7495	346.5764			+ 0.2377
2	React.ord. 1	1.0932	1.0715			6.2497E-2
3	log Kcat 1	0.4500	0.4721			9.0147E-3
4	Area 1/(J/g)	16.5223	16.5223			constant

STATISTICS

Least squares:	1.54803E-2	Number of cycles:	23
Mean of residues:	7.79148E-3	Max.No of cycles:	50
Correlation coefficient:	0.999794	Rel. precision:	0.001000
Durbin-Watson Value:	0.030	t-critical(0.95;192):	1.963
Durbin-Watson Factor:	5.841		

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	192	Cn B					
1	s:	1.75	1.27	193	C1 B					
2	s:	9.26	1.27	194	A3					
3	s:	9.31	1.27	194	A2					
4	s:	9.35	1.27	193	An					



Cycle 16 / Activation energy

NETZSCH Thermokinetics

Date/Time: 03.02.2016 at 13:09

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 255 16.07.2016 18:08:14/Segm.S1/1	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	174.1281	Min. Time/min:	0.0
Max. Temp°C:	227.5372	Max. Time/min:	8.8979
Heating rate/(K/min):	6.002	Sampling time/s:	2.000
Sample mass/mg:	1.310		
Base line type:	tangent area prop.	LeftPts: 70	RightPts: 10

PARAMETERS AND STANDARD DEVIATIONS

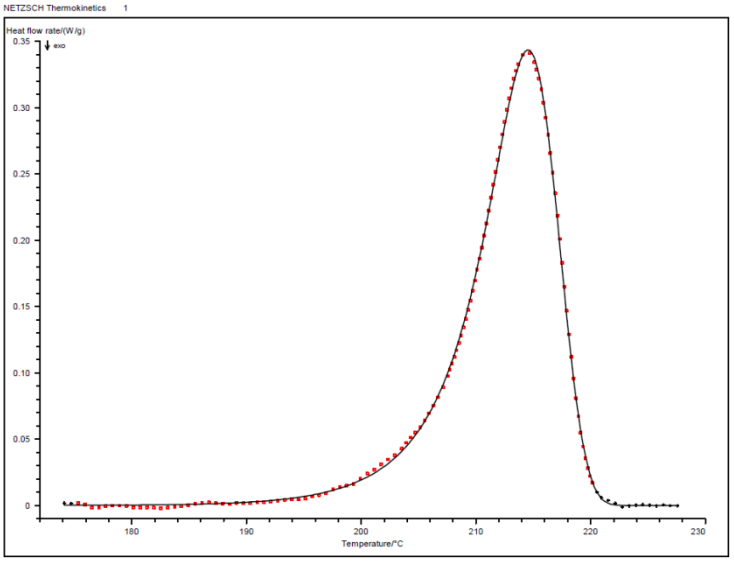
#	Parameter	Initial Val.	Optimum Val.	Minimun	Maximun	Sigrt*Std.Dev.
0	log A1/s^-1	43.0763	37.0889			8.7432E-3
1	E1 kJ/mol	420.2877	365.2751			+ 0.1681
2	React.ord. 1	1.0536	0.9362			5.5884E-2
3	log Kcat 1	0.4500	0.5375			7.8228E-3
4	Area 1/(J/g)	30.9043	30.9043			constant

STATISTICS

Least squares:	1.38443E-2	Number of cycles:	23
Mean of residues:	7.18734E-3	Max.No of cycles:	50
Correlation coefficient:	0.999839	Rel. precision:	0.001000
Durbin-Watson Value:	0.046	t-critical(0.95;224):	1.962
Durbin-Watson Factor:	4.714		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-ac	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.25	224	Cn B					
1	s:	1.80	1.25	225	C1 B					
2	s:	7.36	1.25	225	An					
3	s:	9.45	1.25	225	Fn					
4	s:	9.49	1.25	224	Bna					



Cycle 20 / Activation energy

NETZSCH Thermokinetics

Date/Time: 03.02.2016 at 13:59

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 255 29.07.2015 10:43:36/Segm.S1/1	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	179.7794	Min. Time/min:	0.0
Max. Temp°C:	227.3863	Max. Time/min:	5.2867
Heating rate/(K/min):	9.005	Sampling time/s:	1.333
Sample mass/mg:	1.310		
Base line type:	tangent area prop.	LeftPts: 60	RightPts: 20

PARAMETERS AND STANDARD DEVIATIONS

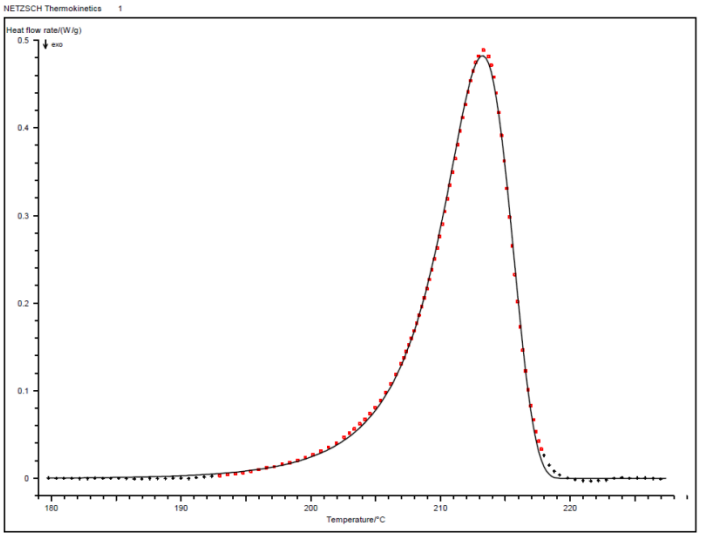
#	Parameter	Initial Val.	Optimum Val.	Minimun	Maximun	Sigrt*Std.Dev.
0	log A1/s^-1	47.1125	36.9533			5.4709E-3
1	E1 kJ/mol	455.0106	362.4580			+ 0.1080
2	React.ord. 1	0.8957	0.8519			4.1742E-2
3	log Kcat 1	0.4500	0.7480			8.3408E-3
4	Area 1/(J/g)	24.4576	24.4576			constant

STATISTICS

Least squares:	4.30614E-2	Number of cycles:	19
Mean of residues:	1.34228E-2	Max.No of cycles:	50
Correlation coefficient:	0.999648	Rel. precision:	0.001000
Durbin-Watson Value:	0.060	t-critical(0.95;123):	1.970
Durbin-Watson Factor:	4.125		

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	1.35	123	Cn B					
1	s:	3.61	1.35	124	C1 B					
2	s:	3.98	1.35	125	D1F					
3	s:	9.57	1.35	125	D3F					
4	s:	10.81	1.35	124	Fn					



Cycle 21 / Activation energy

NETZSCH Thermokinetics

Date/Time: 03.02.2016 at 14:21

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:		Op 255 30.07.2015 11:30:45/Segm.S1/1	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	169.9010	Min. Time/min:	0.0
Max. Temp°C:	227.5113	Max. Time/min:	6.3981
Heating rate/(K/min):	9.004	Sampling time/s:	1.333
Sample mass/mg:	1.310		
Base line type:	tangent area prop.	LeftPts: 50	RightPts: 8

PARAMETERS AND STANDARD DEVIATIONS

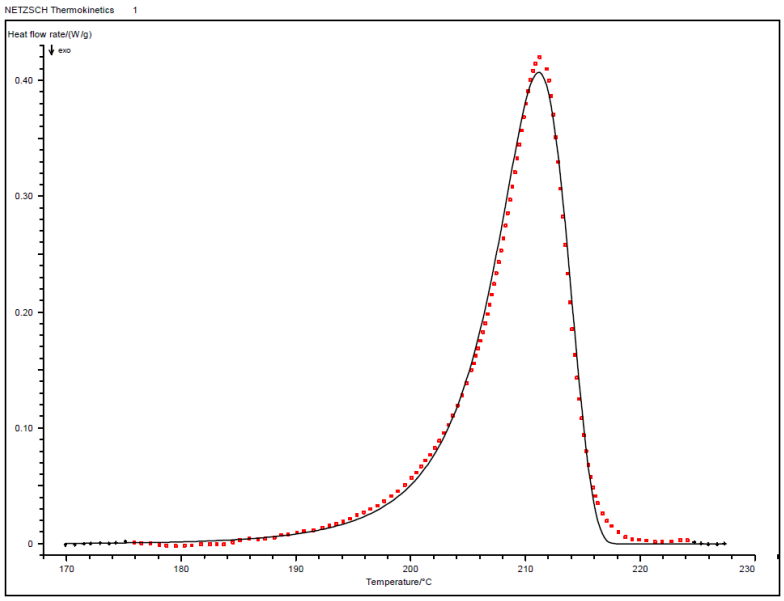
#	Parameter	Initial Val.	Optimum Val.	Minimun	Maximun	Sigrt*	Std.Dev.
0	log A1/s^-1	27.6988	27.6989				0.4440
1	E1 kJ/mol	276.6311	276.6312			+	4.0711
2	React.ord. 1	0.8147	0.8140			+	0.1716
3	log Kcat 1	0.8404	0.8400				5.8158E-2
4	Area 1/(J/g)	24.5259	24.5259				constant

STATISTICS

Least squares:	0.22679	Number of cycles:	11
Mean of residues:	2.80131E-2	Max.No of cycles:	50
Correlation coefficient:	0.997915	Rel. precision:	0.001000
Durbin-Watson Value:	0.031	t-critical(0.95;238):	1.961
Durbin-Watson Factor:	5.708		

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	238	Cn B					
1	s:	1.63	1.24	239	C1 B					
2	s:	2.32	1.24	240	D3F					
3	s:	3.07	1.24	239	An					
4	s:	3.38	1.24	239	Fn					



Cycle 22 / Activation energy

NETZSCH Thermokinetics

Date/Time: 03.02.2016 at 14:24

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 255 31.07.2015 13:08:35/Segm.S1/1	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	176.2536	Min. Time/min:	0.0
Max. Temp°C:	227.4630	Max. Time/min:	5.6880
Heating rate/(K/min):	9.003	Sampling time/s:	1.333
Sample mass/mg:	1.310		
Base line type:	tangent area prop.	LeftPts: 50	RightPts: 7

PARAMETERS AND STANDARD DEVIATIONS

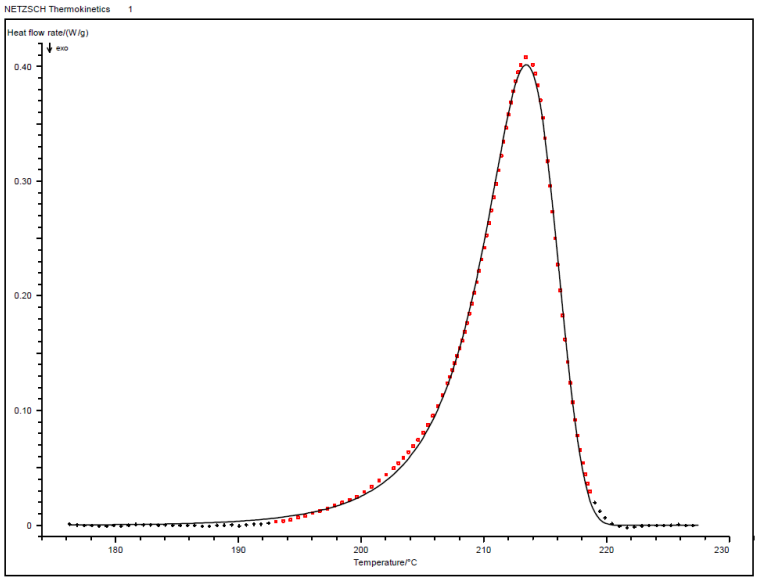
#	Parameter	Initial Val.	Optimum Val.	Minimun	Maximun	Sigrt*	Std.Dev.
0	log A1/s^-1	43.8516	34.3684				1.1414E-2
1	E1 kJ/mol	425.0963	338.6499			+	0.2221
2	React.ord. 1	0.9541	0.8978				8.1385E-2
3	log Kcat 1	0.4500	0.7197				1.1747E-2
4	Area 1/(J/g)	22.8175	22.8175				constant

STATISTICS

Least squares:	4.15463E-2	Number of cycles:	19
Mean of residues:	1.27145E-2	Max.No of cycles:	50
Correlation coefficient:	0.999494	Rel. precision:	0.001000
Durbin-Watson Value:	0.032	t-critical(0.95;126):	1.970
Durbin-Watson Factor:	5.616		

F-TEST ON FIT-QUALITY

#	Code	Fexp	Fcrit(0.95)	f-ac	Type 1	Type 2	Type 3	Type 4	Type 5	Type 6
0	s:	1.00	1.34	126	Cn B					
1	s:	1.89	1.34	127	C1 B					
2	s:	4.95	1.34	128	D1F					
3	s:	7.02	1.34	127	An					
4	s:	8.20	1.34	127	Fn					



Cycle 23 / Activation energy

NETZSCH Thermokinetics

Date/Time: 03.02.2016 at 14:26

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:		Op 255 03.08.2015 14:55:33/Segm.S1/1	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	179.6356	Min. Time/min:	0.0
Max. Temp°C:	227.4468	Max. Time/min:	5.3100
Heating rate/(K/min):	9.004	Sampling time/s:	1.333
Sample mass/mg:	1.310		
Base line type:	tangent area prop.	LeftPts: 50	RightPts: 7

PARAMETERS AND STANDARD DEVIATIONS

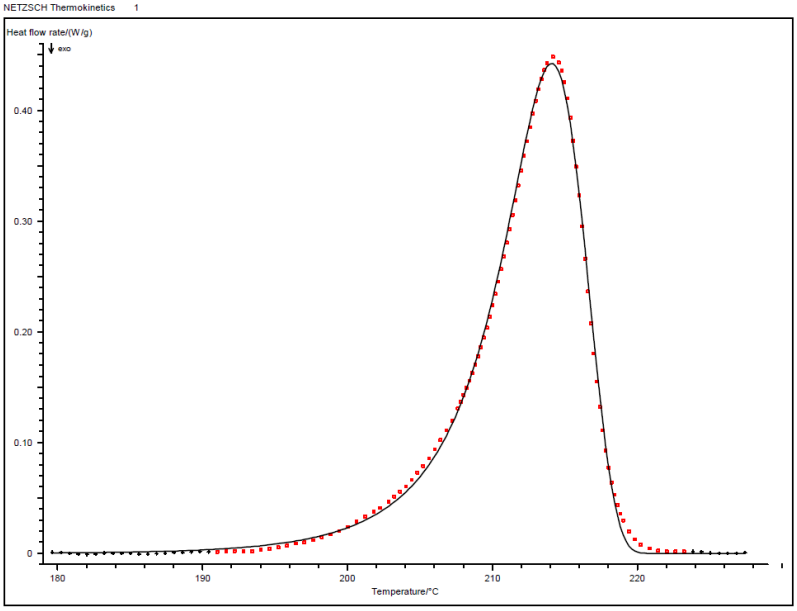
#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sigrt*Std.Dev.
0	log A1/s^-1	42.8485	35.9709			6.1102E-3
1	E1 kJ/mol	416.4318	353.6080			8.0819E-2
2	React.ord. 1	0.8792	0.8550			3.6694E-2
3	log Kcat 1	0.4500	0.6628			1.2388E-2
4	Area 1/(J/g)	24.2074	24.2074			constant

STATISTICS

Least squares:	9.23205E-2	Number of cycles:	19
Mean of residues:	1.96130E-2	Max.No of cycles:	50
Correlation coefficient:	0.999264	Rel. precision:	0.001000
Durbin-Watson Value:	0.038	t-critical(0.95;160):	1.966
Durbin-Watson Factor:	5.169		

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	1.30	160	Cn B					
1	s:	1.54	1.30	162	D1F					
2	s:	2.26	1.30	161	C1 B					
3	s:	3.94	1.30	162	D3F					
4	s:	5.30	1.30	161	Fn					



Cycle 24 / Activation energy

NETZSCH Thermokinetics

Date/Time: 03.02.2016 at 15:19

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 255 04.08.2015 11:55:00/Segm.S1/1	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	165.7738	Min. Time/min:	0.0
Max. Temp°C:	227.1731	Max. Time/min:	5.1130
Heating rate/(K/min):	12.008	Sampling time/s:	0.999
Sample mass/mg:	1.310		
Base line type:	tangent area prop.	LeftPts: 100	RightPts: 1

PARAMETERS AND STANDARD DEVIATIONS

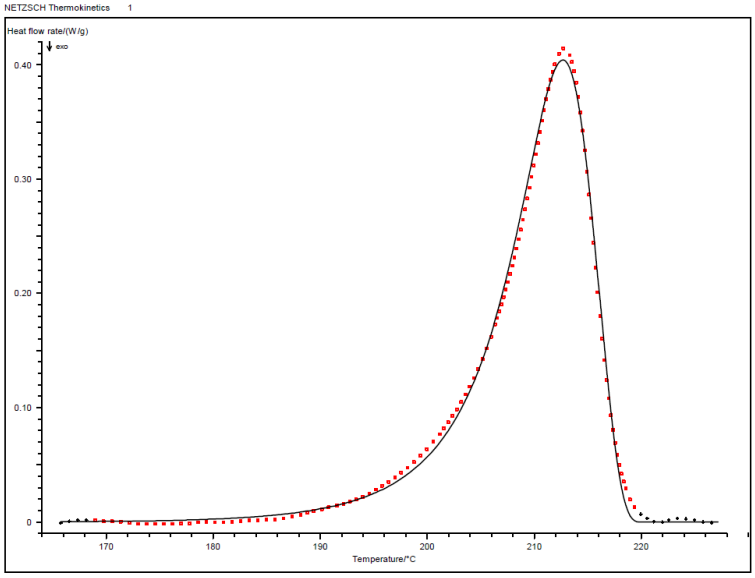
#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sigrt*Std.Dev.
0	log A1/s^-1	30.3269	25.5707			0.3025
1	E1 kJ/mol	299.0150	255.9739			+ 2.7158
2	React.ord. 1	0.7698	0.7866			7.0665E-2
3	log Kcat 1	0.4500	0.6643			4.4024E-2
4	Area 1/(J/g)	21.4900	21.4900			constant

STATISTICS

Least squares:	0.13566	Number of cycles:	16
Mean of residues:	2.09870E-2	Max.No of cycles:	50
Correlation coefficient:	0.998840	Rel. precision:	0.001000
Durbin-Watson Value:	0.023	t-critical(0.95;252):	1.961
Durbin-Watson Factor:	6.650		

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	252	Cn B					
1	s:	2.17	1.23	254	D3F					
2	s:	2.87	1.23	253	C1 B					
3	s:	3.96	1.23	253	Fn					
4	s:	4.15	1.23	254	R3					



Cycle 25 / Activation energy

NETZSCH Thermokinetics

Date/Time: 03.02.2016 at 15:15

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:		Op 255 05.08.2015 11:57:37/Segm.S1/1	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	165.8194	Min. Time/min:	0.0
Max. Temp°C:	227.0363	Max. Time/min:	5.0974
Heating rate/(K/min):	12.009	Sampling time/s:	0.999
Sample mass/mg:	1.310		
Base line type:	tangent area prop.	LeftPts: 102	RightPts: 8

PARAMETERS AND STANDARD DEVIATIONS

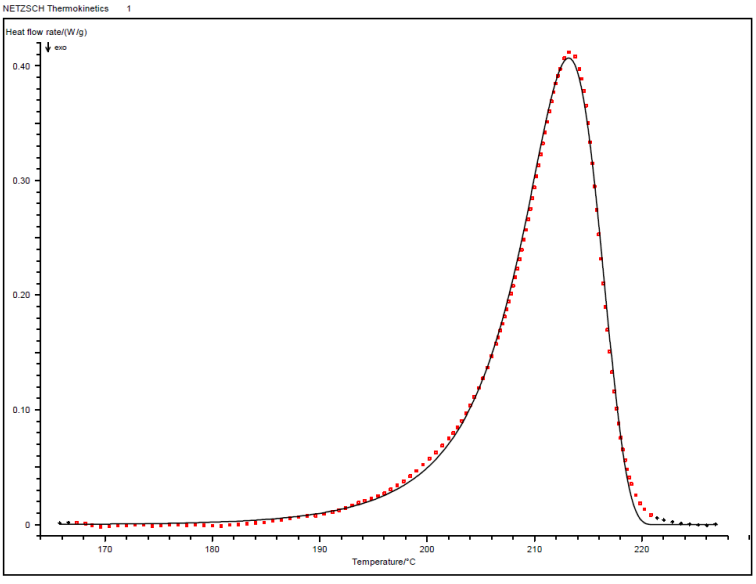
#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sigrt*Std.Dev.
0	log A1/s^-1	26.0358	26.0358			7.9116E-3
1	E1 kJ/mol	260.6830	260.6830			9.6994E-2
2	React.ord. 1	0.8251	0.8251			4.0280E-2
3	log Kcat 1	0.7050	0.7050			1.3091E-2
4	Area 1/(J/g)	21.3817	21.3817			constant

STATISTICS

Least squares:	8.85862E-2	Number of cycles:	14
Mean of residues:	1.69869E-2	Max.No of cycles:	50
Correlation coefficient:	0.999268	Rel. precision:	0.001000
Durbin-Watson Value:	0.025	t-critical(0.95;267):	1.960
Durbin-Watson Factor:	6.340		

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	267	Cn B					
1	s:	2.70	1.22	268	C1 B					
2	s:	3.35	1.22	269	D3F					
3	s:	5.29	1.22	268	Fn					
4	s:	6.14	1.22	269	R3					



Cycle 26/ Activation energy

NETZSCH Thermokinetics

Date/Time: 03.02.2016 at 14:55

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 255 06.08.2015 12:11:54/Segm.S1/1	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	169.9803	Min. Time/min:	0.0
Max. Temp°C:	227.3754	Max. Time/min:	4.7818
Heating rate/(K/min):	12.003	Sampling time/s:	1.000
Sample mass/mg:	1.310		
Base line type:	tangent area prop.	LeftPts: 7	RightPts: 8

PARAMETERS AND STANDARD DEVIATIONS

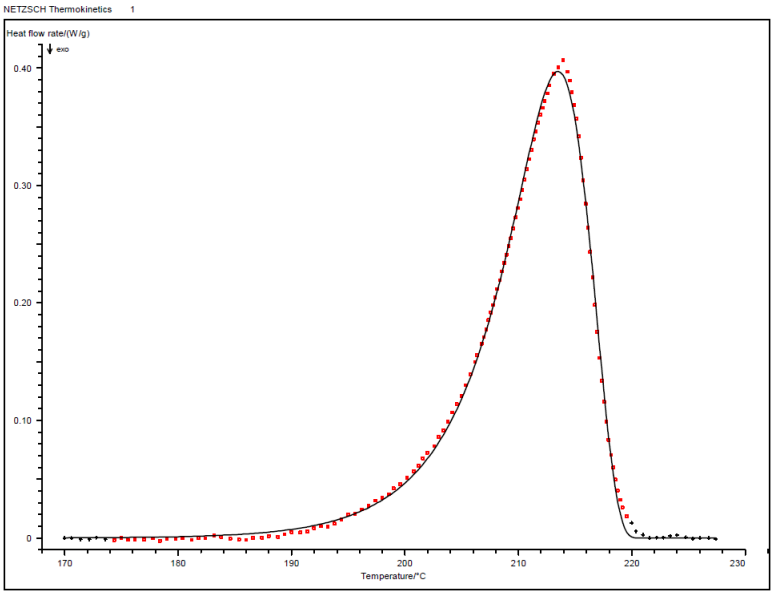
#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sigrt*Std.Dev.
0	log A1/s^-1	24.3838	33.7261			8.0300E-3
1	E1 kJ/mol	244.5840	329.6794			+ 0.1079
2	React.ord. 1	0.6657	0.7978			4.0140E-2
3	log Kcat 1	0.4500	0.2450			2.1284E-2
4	Area 1/(J/g)	20.7742	20.7742			constant

STATISTICS

Least squares:	7.18487E-2	Number of cycles:	23
Mean of residues:	1.57948E-2	Max.No of cycles:	50
Correlation coefficient:	0.999393	Rel. precision:	0.001000
Durbin-Watson Value:	0.057	t-critical(0.95;226):	1.962
Durbin-Watson Factor:	4.216		

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	226	Cn B					
1	s:	1.23	1.25	228	D3F					
2	s:	1.34	1.25	228	D1F					
3	s:	3.16	1.25	227	Fn					
4	s:	3.58	1.25	228	R3					



Cycle 27 / Activation energy

NETZSCH Thermokinetics

Date/Time: 03.02.2016 at 15:24

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 255 07.08.2015 15:45:53/Segm.S1/1	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	167.2805	Min. Time/min:	0.0
Max. Temp°C:	227.2853	Max. Time/min:	4.9974
Heating rate/(K/min):	12.007	Sampling time/s:	0.999
Sample mass/mg:	1.310		
Base line type:	tangent area prop.	LeftPts: 100	RightPts: 8

PARAMETERS AND STANDARD DEVIATIONS

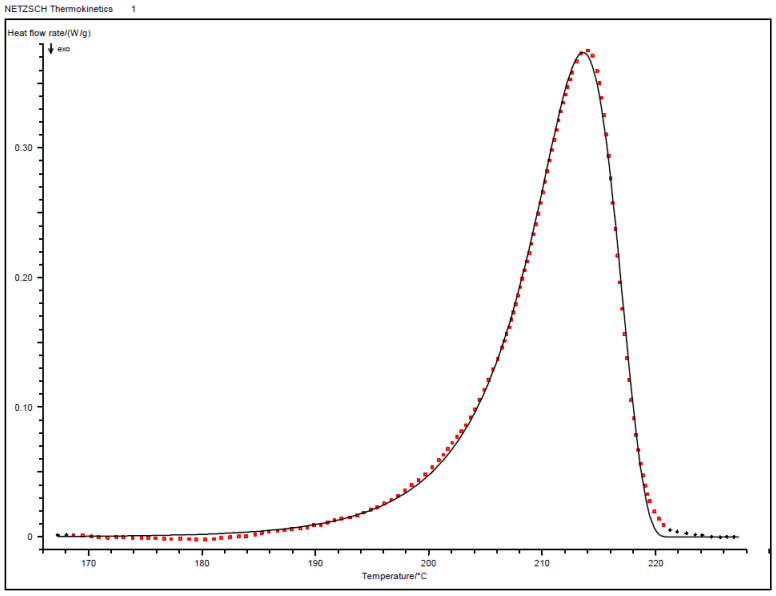
#	Parameter	Initial Val.	Optimum Val.	Minimun	Maximun	Sigrt*	Std.Dev.
0	log A1/s^-1	27.1547	27.6357				0.2931
1	E1 kJ/mol	270.2481	274.7465			+	2.6482
2	React.ord. 1	0.7478	0.7946				5.4682E-2
3	log Kcat 1	0.4500	0.5164				3.8482E-2
4	Area 1/(J/g)	20.2956	20.2956				constant

STATISTICS

Least squares:	5.96914E-2	Number of cycles:	18
Mean of residues:	1.40822E-2	Max.No of cycles:	50
Correlation coefficient:	0.999438	Rel. precision:	0.001000
Durbin-Watson Value:	0.035	t-critical(0.95;259):	1.960
Durbin-Watson Factor:	5.332		

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	259	Cn B					
1	s:	2.21	1.23	261	D3F					
2	s:	4.54	1.23	260	C1 B					
3	s:	4.92	1.23	260	Fn					
4	s:	5.32	1.23	261	R3					



Cycle 31 / Activation energy

NETZSCH Thermokinetics

Date/Time: 17.02.2016 at 16:17

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:		Op 255 25.01.2016 11:29:15/Segm.S1/2	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	170.6458	Min. Time/min:	0.0
Max. Temp°C:	227.6546	Max. Time/min:	6.3314
Heating rate/(K/min):	9.004	Sampling time/s:	1.333
Sample mass/mg:	1.310		
Base line type:		LeftPts: 40	RightPts: 20

PARAMETERS AND STANDARD DEVIATIONS

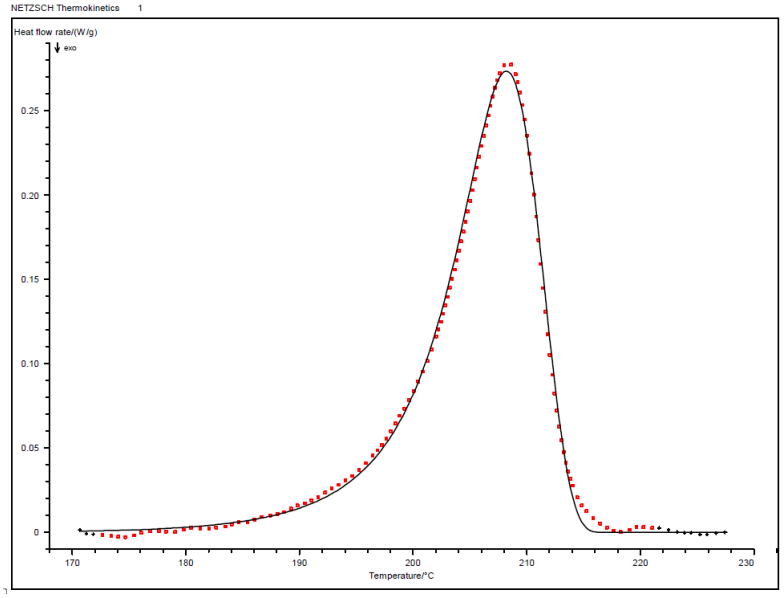
#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sigrt*Std.Dev.
0	log A1/s^-1	32.4585	25.3935			1.0839E-2
1	E1 kJ/mol	316.6782	253.3513			+ 0.1381
2	React.ord. 1	0.8798	0.8454			5.5051E-2
3	log Kcat 1	0.4500	0.7229			1.6025E-2
4	Area 1/(J/g)	19.3019	19.3019			constant

STATISTICS

Least squares:	5.86902E-2	Number of cycles:	19
Mean of residues:	1.43251E-2	Max.No of cycles:	50
Correlation coefficient:	0.998946	Rel. precision:	0.001000
Durbin-Watson Value:	0.023	t-critical(0.95;240):	1.961
Durbin-Watson Factor:	6.610		

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	240	Cn B					
1	s:	1.10	1.24	242	D1F					
2	s:	1.90	1.24	241	C1 B					
3	s:	3.04	1.24	242	D3F					
4	s:	4.35	1.24	241	Fn					



Cycle 33 / Activation energy

NETZSCH Thermokinetics

Date/Time: 17.02.2016 at 16:22

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:		Op 255 09.02.2016 14:35:23/Segm.S1/2	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	178.9042	Min. Time/min:	0.0
Max. Temp°C:	227.7066	Max. Time/min:	5.4200
Heating rate/(K/min):	9.004	Sampling time/s:	1.333
Sample mass/mg:	1.310		
Base line type:		LeftPts: 7	RightPts: 7

PARAMETERS AND STANDARD DEVIATIONS

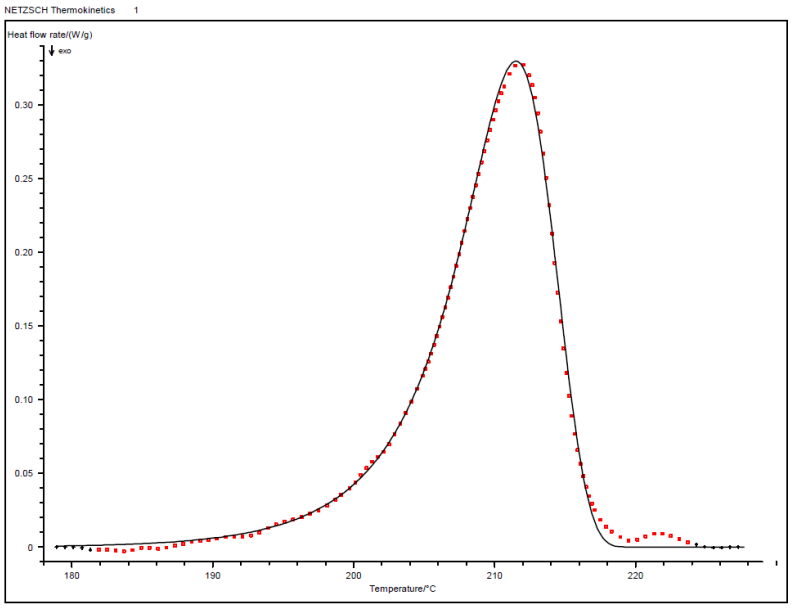
#	Parameter	Initial Val.	Optimum Val.	Minimun	Maximun	Sigrt*Std.Dev.
0	log A1/s^-1	31.9239	34.2584			9.7746E-3
1	E1 kJ/mol	313.7417	335.2166			+ 0.1397
2	React.ord. 1	0.8398	0.8801			5.3690E-2
3	log Kcat 1	0.4500	0.4918			1.7832E-2
4	Area 1/(J/g)	20.9336	20.9336			constant

STATISTICS

Least squares:	7.67039E-2	Number of cycles:	22
Mean of residues:	1.76940E-2	Max.No of cycles:	50
Correlation coefficient:	0.999094	Rel. precision:	0.001000
Durbin-Watson Value:	0.036	t-critical(0.95;208):	1.963
Durbin-Watson Factor:	5.327		

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:	1.64	1.26	209	C1 B					
2	s:	2.10	1.26	210	D1F					
3	s:	2.67	1.26	210	D3F					
4	s:	3.16	1.26	209	Fn					



Cycle 35 / Activation energy

NETZSCH Thermokinetics

Date/Time: 17.02.2016 at 16:14

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 255 15.02.2016 11:04:33/Segm.S1/1	
Transfer Corr:	204_F1.kcr		
Min. Temp/°C:	168.3587	Min. Time/min:	0.0
Max. Temp°C:	227.7710	Max. Time/min:	6.5989
Heating rate/(K/min):	9.003	Sampling time/s:	1.333
Sample mass/mg:	1.310		
Base line type:		LeftPts: 40	RightPts: 20

PARAMETERS AND STANDARD DEVIATIONS

#	Parameter	Initial Val.	Optimum Val.	Minimum	Maximum	Sigrt*Std.Dev.
0	log A1/s^-1	24.3825	27.8470			1.4435E-2
1	E1 kJ/mol	244.0075	275.0898			+ 0.2078
2	React.ord. 1	0.8846	0.9221			5.8005E-2
3	log Kcat 1	0.4500	0.3416			1.3331E-2
4	Area 1/(J/g)	19.6107	19.6107			constant

STATISTICS

Least squares:	8.34402E-3	Number of cycles:	22
Mean of residues:	5.29151E-3	Max.No of cycles:	50
Correlation coefficient:	0.999784	Rel. precision:	0.001000
Durbin-Watson Value:	0.013	t-critical(0.95;207):	1.963
Durbin-Watson Factor:	8.953		

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:	2.42	1.26	208	C1 B					
2	s:	8.24	1.26	208	Fn					
3	s:	11.82	1.26	209	D1F					
4	s:	12.62	1.26	209	D3F					

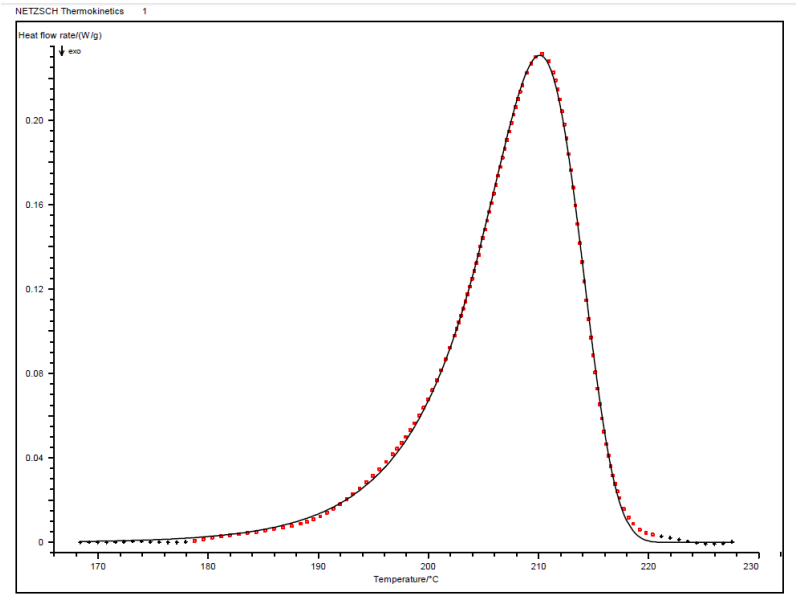


Table S1 Kinetic data for the $\mathbf{1}^{A/LS} \rightarrow \mathbf{1}^{A/HS}$ spin transition used for statistical treatment.

Sample / cycle	*T* / K	ln*k*
14-1 8up	490	-5,84031071006496
14-1 10up	490	-6,20593403052753
14-1 11up	490	-5,96103575448239
14-1 12up	480	-8,71262831901017
14-1 13up	480	-8,2286500400255
14-1 14up	470	-10,5888404984096
9 9up	490	-5,48416574742023
9 10up	490	-6,6346868462134
9 11up	490	-5,57889824174886
9 12up	490	-6,52277880883521
9 13up	490	-6,02208370503121
9 15up	490	-6,49910948319672
9 16up	490	-5,57404085879939
9 17up	490	-5,231248079223
9 18up	490	-6,29174697676658
9 19up	490	-6,02351691084237
9 20up	486	-7,13140358649842
9 21up	486	-6,91725149236731
9 22up	490	-6,64243541052565
9 23up	490	-6,1302644437726
9 24up	482	-8,16959145138272
9 25up	482	-7,39591260206566
9 26up	488	-6,43992377990681
9 27up	488	-5,95110743785233
9 29up	486	-7,06430816070237
9 30up	486	-6,3500712174346
9 31up	486	-5,94771094001058
9 32up	482	-7,95011388521457
9 33up	482	-7,34016942269996
9 35up	484	-7,57335126044111
9 36up	484	-6,9161212105586
4 3up	490	-6,05392950616651
4 4up	486	-5,86788686302251
4 5up	481	-6,53206813716982
4 6up	480	-6,79749653717208
4 7up	480	-6,03760876988061
4 8up	480	-6,85222432078106
4 9up	480	-6,73902939576851
4 11up	476	-6,78950247316817
4 12up	476	-6,60925847799666
4 14up	476	-7,28012201817765
4 15up	476	-7,19987301770959
4 16up	476	-7,18177539254028
4 18up	476	-6,91467660891807
4 19up	476	-6,96945581500806

5-1 4up	490	-5,96378295969458
5-1 5up	486	-6,17323681761731
5-1 6up	482	-7,23978905220486
5-1 7up	482	-7,60498546822286
5-1 8up	482	-7,7995676943524
5-1 9up	486	-7,50924566326606
5-1 10up	486	-7,17641626162313
5-1 11up	486	-7,50653845111657
5-1 13up	486	-7,44486388227383
5-1 14up	486	-7,63355458874244
7 2up	490	-6,59463770970799
7 3up	490	-6,07681767844366
7 4up	480	-6,44103629288871
7 5up	472	-6,98428555438464
7 6up	472	-6,92861294503387
7 9up	460	-7,29846786232034
7 10up	460	-8,00741111423426
7 11up	460	-7,95373919263168
7 12up	460	-7,87299751193767
3 3up	467	-7,09437069736075
3 4up	450	-7,40546586662822
3 5up	450	-7,66862748411647
3 6up	467	-6,50999880441026
3 7up	450	-7,32391482934197
3 8up	440	-7,78614959283031
3 9up	467	-6,55081390262655
3 11up	450	-7,37041027790588
3 12up	450	-6,4749953855373
3 16up	450	-7,24965361365363
3 17up	450	-7,47644458704323
1 2up	400	-5,1760249050894
1 3up	395	-5,61752142129896
1 4up	399	-5,25830122391698
1 5up	395	-5,96224850601522
1 8up	397	-6,03568446581141
1 11up	397	-6,00208784801065