

U1-723

3



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GEOLAB	93.20
Kopi nr.	6
Antall kopier	10

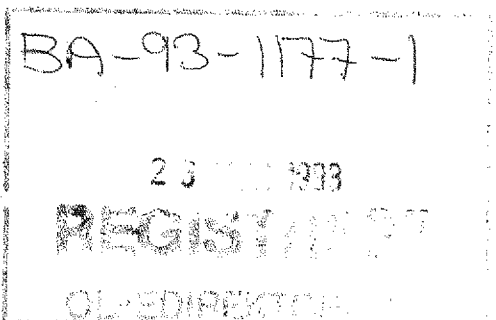
SEKTOR FOR PETROLEUMSTEKNOLOGI
Geologisk laboratorium

Gradering fortrolig

Tittel KINETISKE PARAMETERE FOR DRAUPNEFORMASJONEN I 34/10-36.		
Oppdragsgiver UND GEO/OP	Prosjekt	
Dato 19.02.93	Antall sider 73	Antall vedlegg

Stikkord Kinetiske parametere, TOC, THA, kerogensammensetning

Sammendrag Denne datarapporten presenterer resultater fra kinetiske målinger, TOC- og THA-analyser, samt kvalitativ beskrivelse av kerogensammensetningen for prøver fra Draupneformasjonen i 34/10-36.



Utarbeidet av Kjersti Knudsen Anne Beth Fløtre Åsa Knudsen Lab Instruments Inc.
Tekstoperatør Kjersti Knudsen

Godkjent av
 22/2/93 Ger van Graas
 Ger van Graas, seksjonsleder
 Organisk geokjemi
 23/2-93 Trygve Meyer
 Trygve Meyer, avdelingsleder
 Geologisk laboratorium

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1 INNLEDNING

Dette er en datarapport som presenterer resultater i forbindelse med beregning av kinetiske parametere for Draupneformasjonen i 34/10-36 ved bruk av Pyromat II.

TOC og THA analyser ble foretatt på 8 kjerneprøver og 2 sideveggskjerner (Tabell 1). På grunnlag av disse dataene ble 4 prøver valgt ut til analyse for beregning av kinetiske parametere (jfr. Tabell 3). To paralleller av hver prøve, samt en standardprøve, ble sendt konsulent (Lab Instruments Inc.) for kinetiske målinger ved bruk av Pyromat II. Resultatene er gitt i appendiks. De fire utvalgte prøvene ble petrologisk evaluert for beskrivelse av kerogensammensetning (Tabell 2).

TABELL 1 TOC OG THA DATA FOR DRAUPNEFORMASJONSPRØVER FRA 34/10-36.

DYP mRKB	PRØVE nr.	PRØVE- TYPE	LITOLOGI	S1	S2	TOC	HI	PP	PI	TMAX
3029.25	S6511	core	clyst, olv blk	2.3	29.2	4.5	649	31.5	0.07	421
3030.80	S6512	"	"	3.1	30.9	4.9	631	34.0	0.09	422
3033.50	S6513	"	"	2.6	38.5	5.6	688	41.1	0.06	422
3037.35	S6514	"	"	2.7	29.8	4.8	621	32.5	0.08	421
3039.55	S6515	"	"	3.9	50.2	7.1	707	54.1	0.07	425
3042.00	S6516	"	"	3.6	46.8	6.1	767	50.4	0.07	424
3043.80	S6517	"	"	4.8	33.8	5.2	650	38.6	0.12	420
3047.95	S6518	"	"	4.6	42.9	6.1	703	47.5	0.10	425
3050.50	S6519	"	"	7.4	36.3	6.3	576	43.7	0.17	421
3052.25	S6520	"	"	4.6	53.9	6.6	817	58.5	0.08	428
3117.00	S6521	swc	brn blk	4.0	22.1	6.7	330	26.1	0.15	415
3120.00	S6522	"	"	3.8	18.7	6.3	297	22.5	0.17	415

TABELL 2 BESKRIVELSE¹ AV KEROGENSAMMENSETNINGEN FOR UTVALGTE PRØVER.

S nr.	DYP mRKB	LIPTI- NITT	VITRI- NITT	INERTI- NITT	Kommentarer
S6548	3030.80	xxx	x	x	Liptinitt: dominert av liptodetrinitt, en god del alginitt, noe bituminitt og sporinitt
S6555	3050.50	xxx	x	x	Liptinitt: dominert av liptodetrinitt, mye alginitt, en del bituminitt
S6556	3052.25	xxxx	-	x	Liptinitt: dominert av liptodetrinitt, mye alginitt, en del bituminitt
S6521	3117	xxx	-	xx	Liptnitt: dominert av liptodetrinitt, en god del alginitt, sporinitt og bituminitt

¹ antall x: angir relativ opptreden av de tre maseralgruppene
 -: angir at maseraler innen denne gruppen er observert

TABELL 3 IDENTIFIKASJON AV PRØVER VALGT
FOR KINETISKE BEREGNINGER.

PRØVE NR. hos Lab Instr.	S NR.	DYP mRKB
Sample 361	S6548	3030.80
" 362	S6555	3050.50
" 363	S6556	3052.25
" 364	S6521	3117
" 365	-	STD
" 366	S6548	3030.80
" 367	S6555	3050.50
" 368	S6556	3052.25
" 369	S6521	3117

APPENDIKS

KINETIC ANALYSES

Lab Instruments Inc., January, 1993

T. 183002

KINETIC ANALYSES

SAMPLES 361 TO 369

JANUARY, 1993

LAB INSTRUMENTS, INC.
332 GREENE ST., P.O. BOX# 60,
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KINETIC ANALYSES

SAMPLES 361 TO 369

JANUARY, 1993

LAB INSTRUMENTS, INC.
332 GREENE ST., P.O. BOX# 60,
KENWOOD, CA 95452 U.S.A.

Kenwood 13. JANUARY 1993

Kinetic analysis on 9 whole rocks from STATOIL

- Samples were analyzed on a PYROMAT II micropyrolyzer.
- Kinetic factors computation was done with the KINETICS program developed at L.L.N.L.
- Temperature programming:
10 minutes at 250 Deg.C. then pyrolysis up to 700 deg.C (650 for 1 deg/min. heating rate.)
- Heating rates: About 50,5 and 1 Deg./minute, Up to 3 experiments for HR=50.
- Samples weight: between 10 and 100 mg. depending of sample and heating rate.
- 500 data points collected, data reduction to about 100 points with high and low temperature limits, baseline correction and smoothing.
- KINETICS computation mode: Discrete with 1000 Cal/Mole step.
- Report with KINWIN software.

All samples have correct frequency factors.

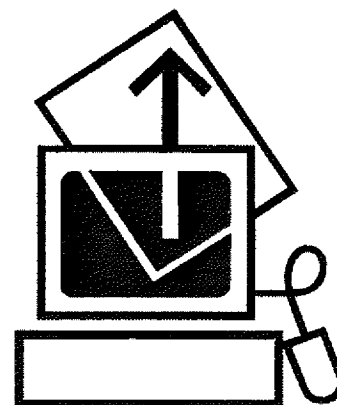
Alain M. Samoun President

Tech Report KINETIC ANALYSES

LAB INSTRUMENTS Inc.

332 Greene St.
P.O. Box #60
KENWOOD
Ca 95452 U.S.A.

Tel/Fax:
(1) 707 833 2038

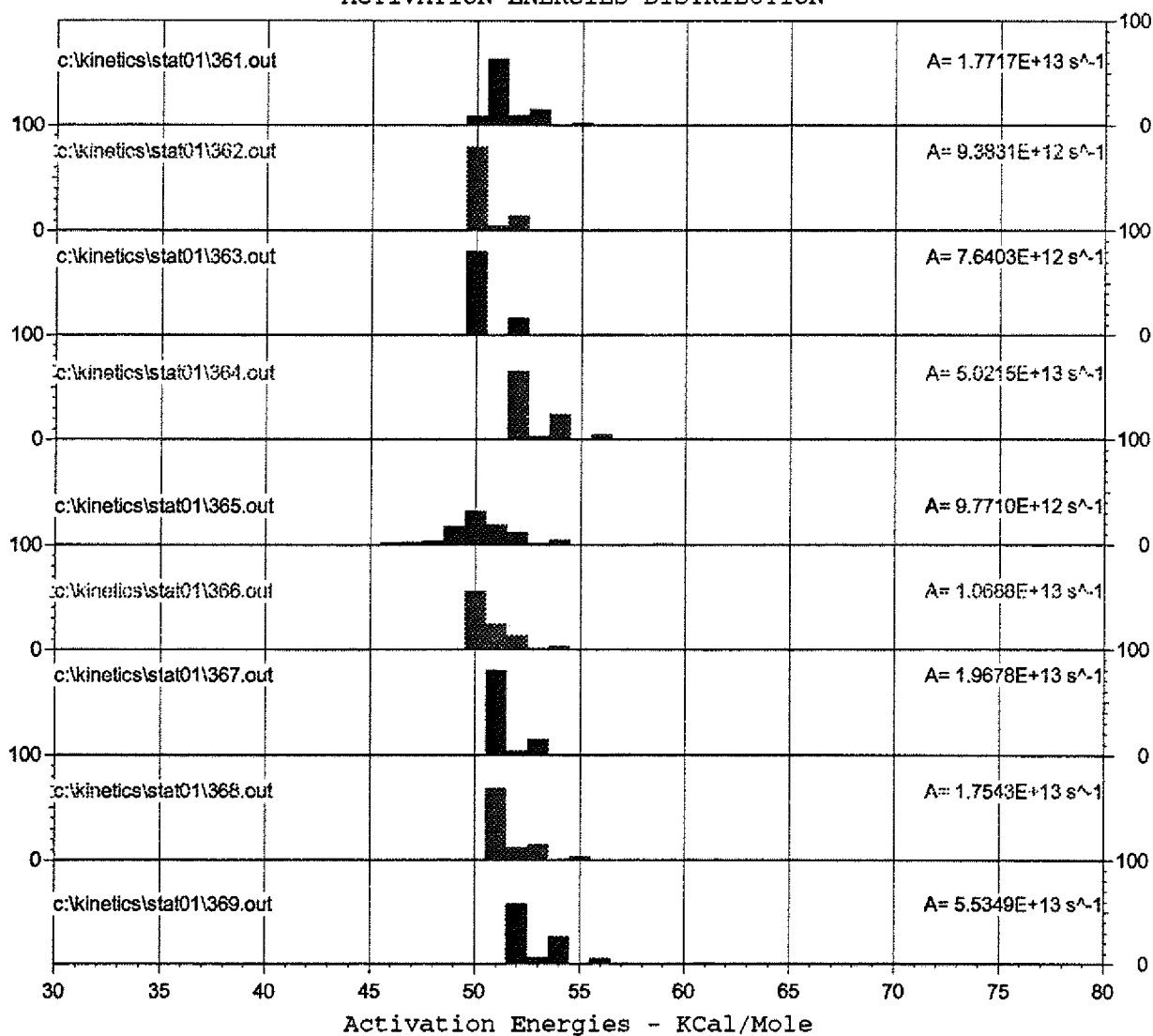


KINETICS FOR WINDOWS

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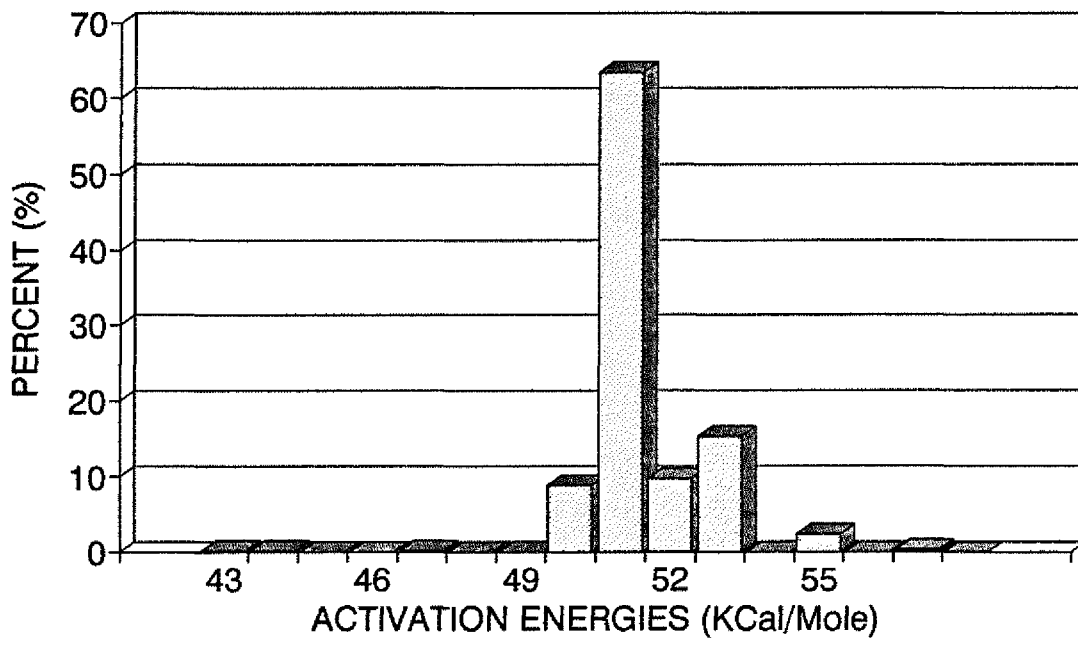
c:\kinetics\stat01\361.out - A=1.7717E+13 s^-1
c:\kinetics\stat01\362.out - A=9.3831E+12 s^-1
c:\kinetics\stat01\363.out - A=7.6403E+12 s^-1
c:\kinetics\stat01\364.out - A=5.0215E+13 s^-1
c:\kinetics\stat01\365.out - A=9.7710E+12 s^-1
c:\kinetics\stat01\366.out - A=1.0688E+13 s^-1
c:\kinetics\stat01\367.out - A=1.9678E+13 s^-1
c:\kinetics\stat01\368.out - A=1.7543E+13 s^-1
c:\kinetics\stat01\369.out - A=5.5349E+13 s^-1
    
```

ACTIVATION ENERGIES DISTRIBUTION



ACTIVATION ENERGIES DISTRIBUTION

Sample 361



Frequency factor = $1.7717E+13 \text{ s}^{-1}$

Sample 361

Fitting method: Discrete (option 1)
Least squares of: Relative Rates
Error tolerance for initial search: 1.0000E-01
Error tolerance for final convergence: 1.0000E-02
Thermal history: Constant heating rate (max. rel. std. dev. =

Initial minimum frequency factor(s^{-1}): 6.8318E+11

Initial maximum frequency factor(s^{-1}): 6.8318E+13

Results

Frequency factor = 1.7717E+13 s^{-1}

Percent	Activation energy (cal/mol)
.09	43000.
.10	44000.
.00	45000.
.00	46000.
.07	47000.
.00	48000.
.00	49000.
8.85	50000.
63.51	51000.
9.58	52000.
15.30	53000.
.00	54000.
2.23	55000.
.00	56000.
.28	57000.

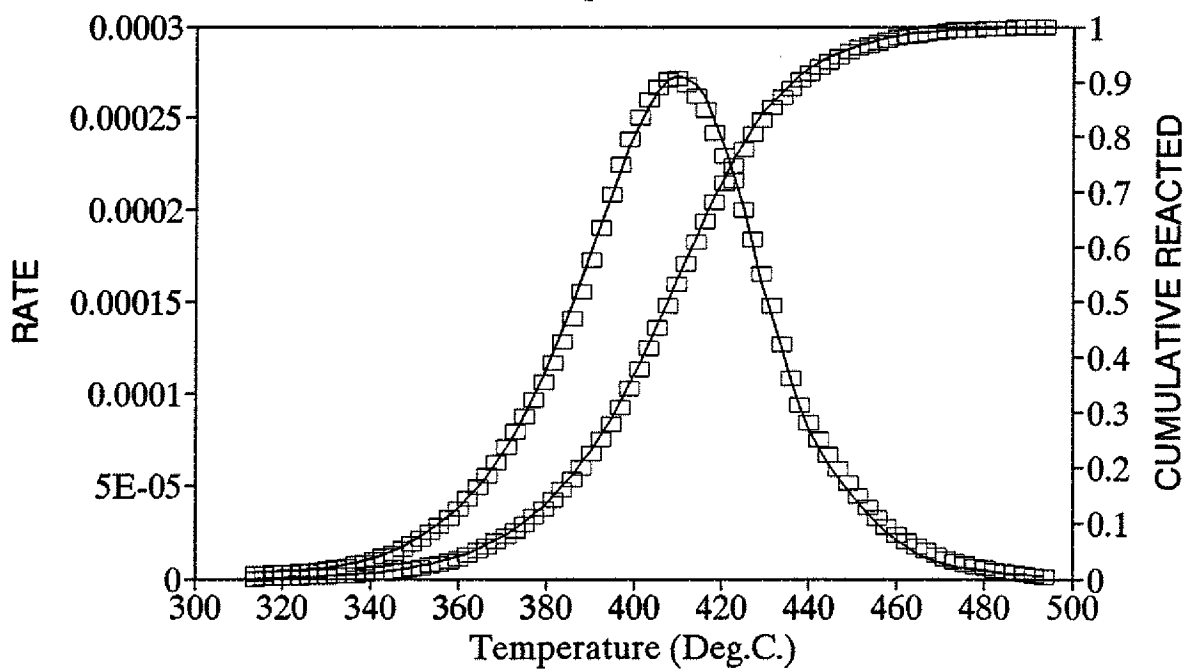
Least squares exit: successful completion

Sum of squares of weighted normalized rate residuals: 6.0275E-02

Sum of squares of weighted integrated rate residuals: 1.2208E-02

EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 361

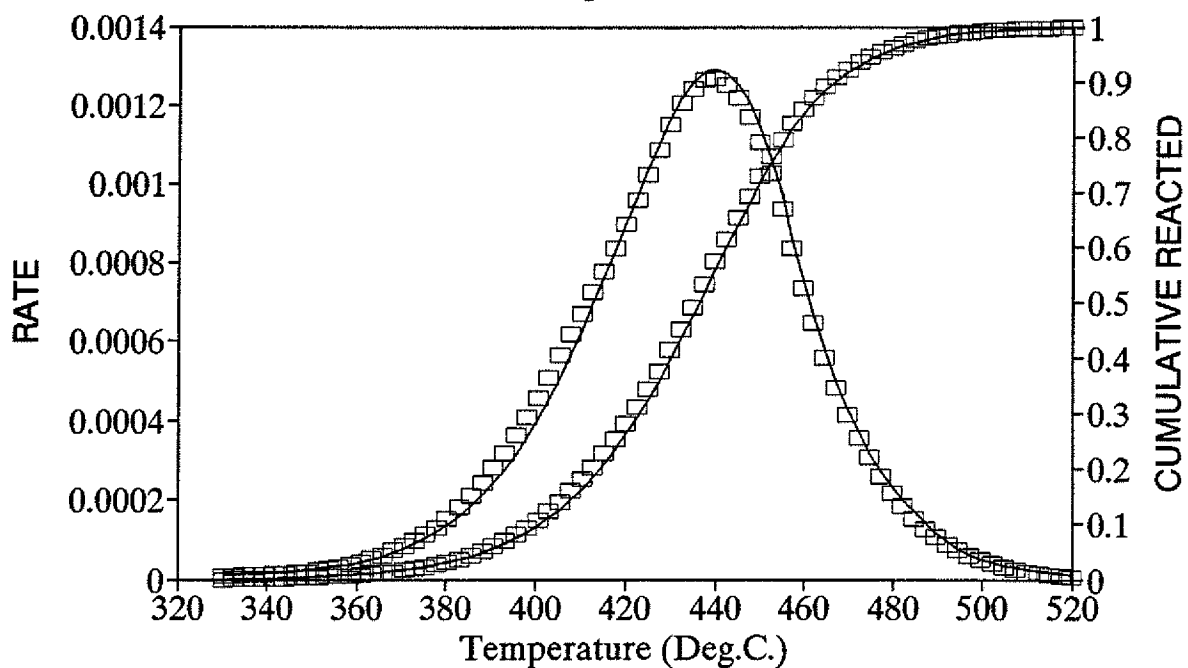


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— COMPUTED

EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 361

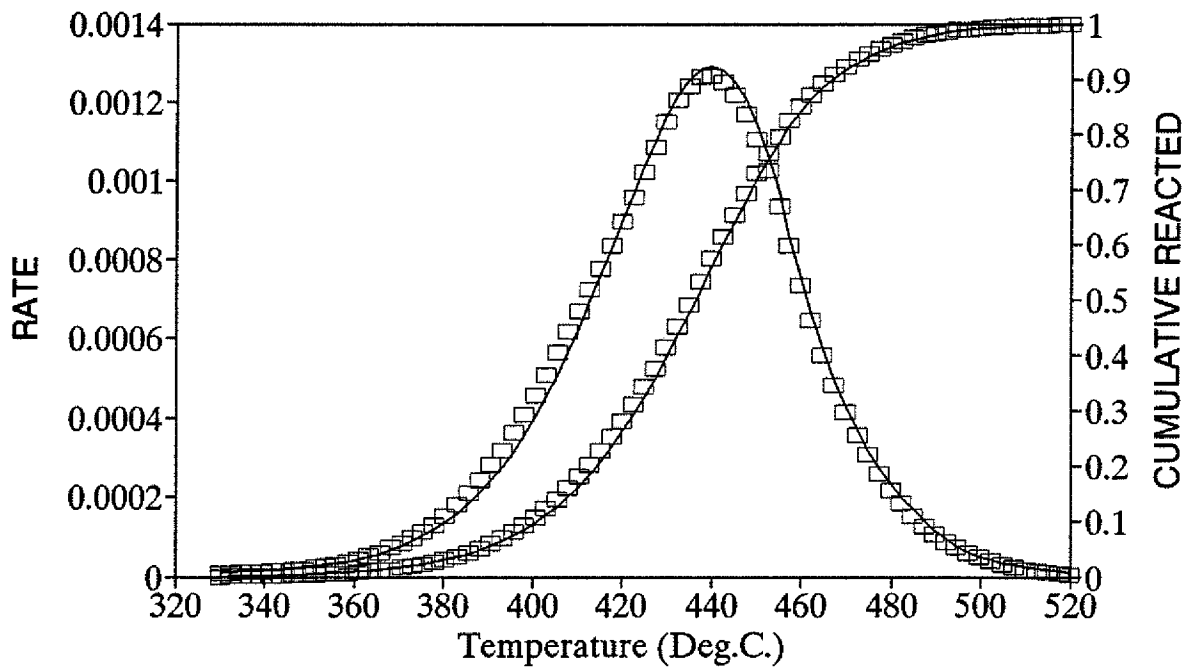


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EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 361

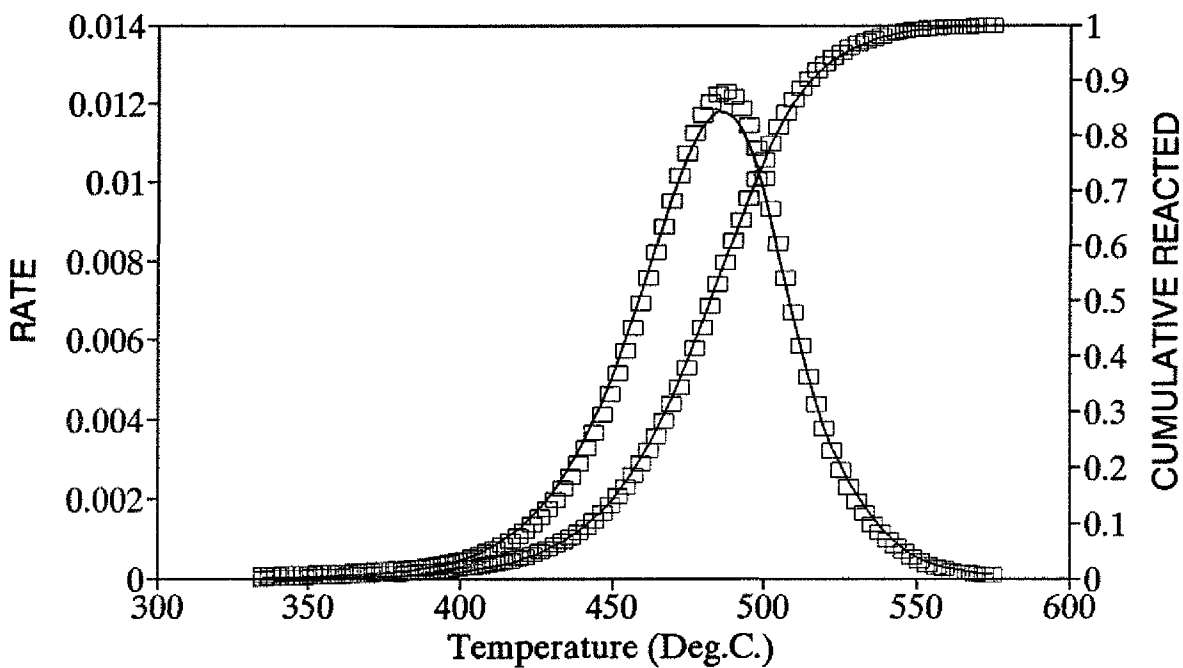


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EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 361

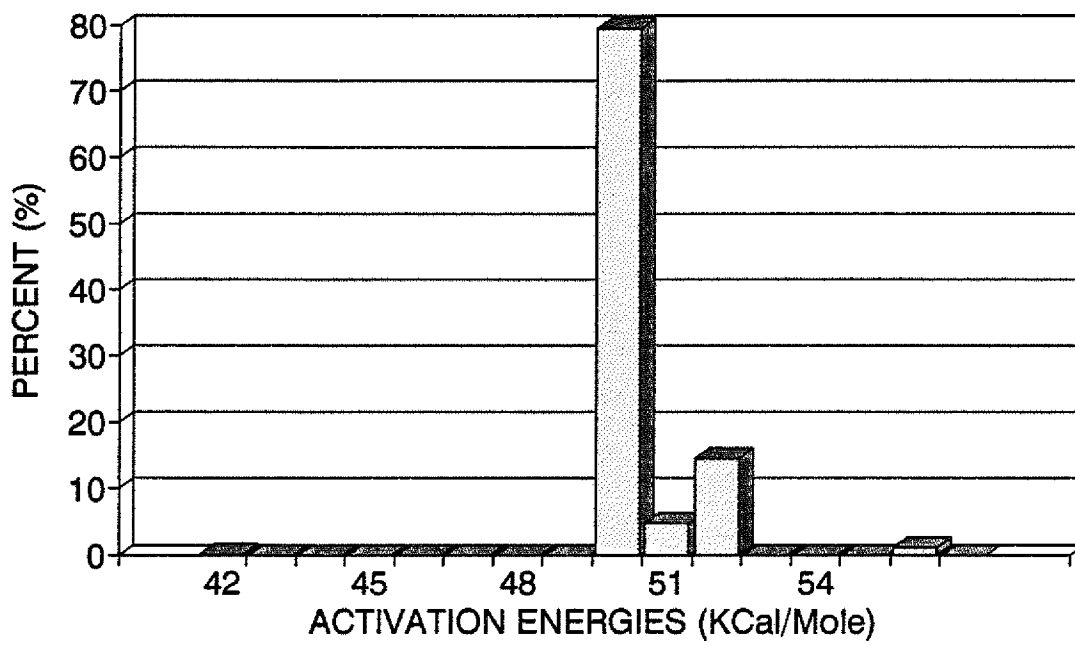


□ c:\kinetics\stat01\36150.prn

— COMPUTED

ACTIVATION ENERGIES DISTRIBUTION

Sample 362



Frequency factor = $9.3831E+12 \text{ s}^{-1}$

Sample 362

Fitting method: Discrete (option 1)
Least squares of: Relative Rates
Error tolerance for initial search: 1.0000E-01
Error tolerance for final convergence: 1.0000E-02
Thermal history: Constant heating rate (max. rel. std. dev. =

Initial minimum frequency factor(s⁻¹): 2.1215E+11
Initial maximum frequency factor(s⁻¹): 2.1215E+13

Results

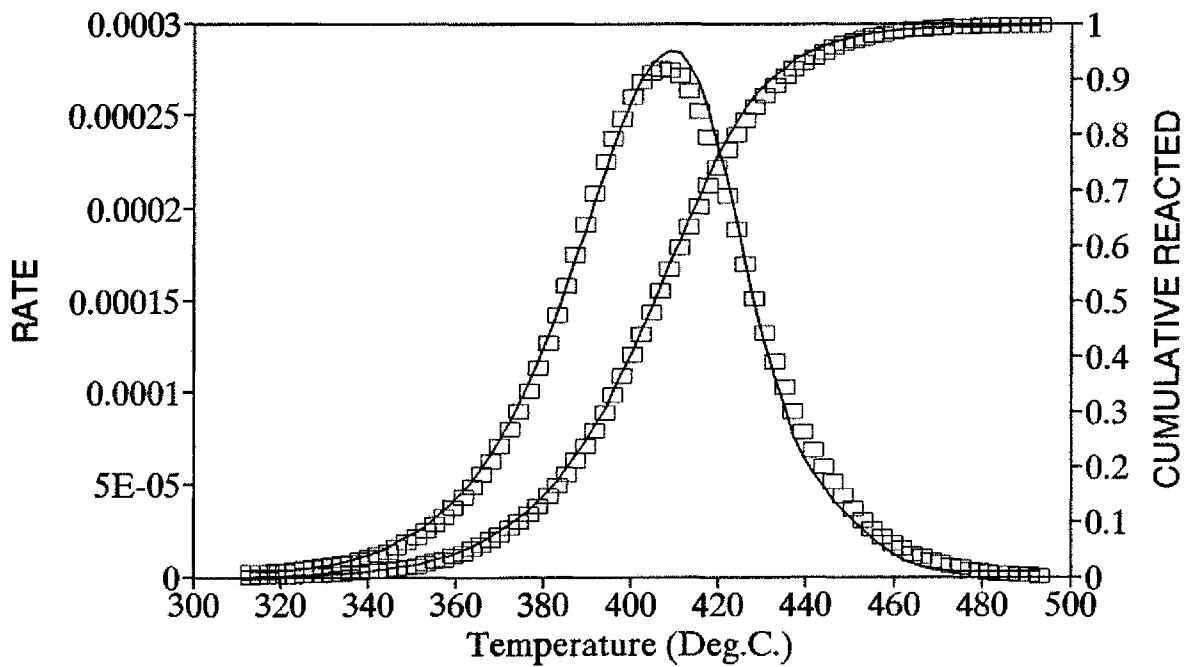
Frequency factor = 9.3831E+12 s⁻¹
Percent Activation energy (cal/mol)

.05	42000.
.00	43000.
.00	44000.
.00	45000.
.00	46000.
.00	47000.
.00	48000.
.00	49000.
79.50	50000.
4.85	51000.
14.56	52000.
.00	53000.
.00	54000.
.00	55000.
1.05	56000.

Least squares exit: successful completion
Sum of squares of weighted normalized rate residuals: 1.7182E-01
Sum of squares of weighted integrated rate residuals: 2.0263E-02

EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 362

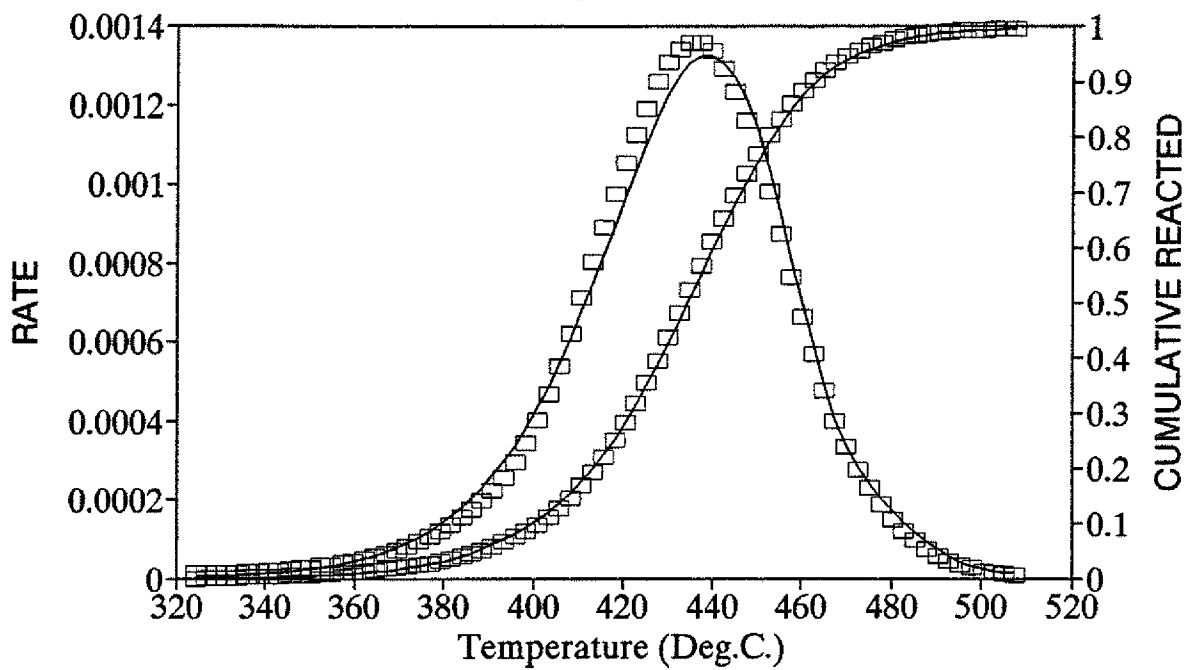


□ c:\kinetics\stat01\36201.prn

— COMPUTED

EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 362

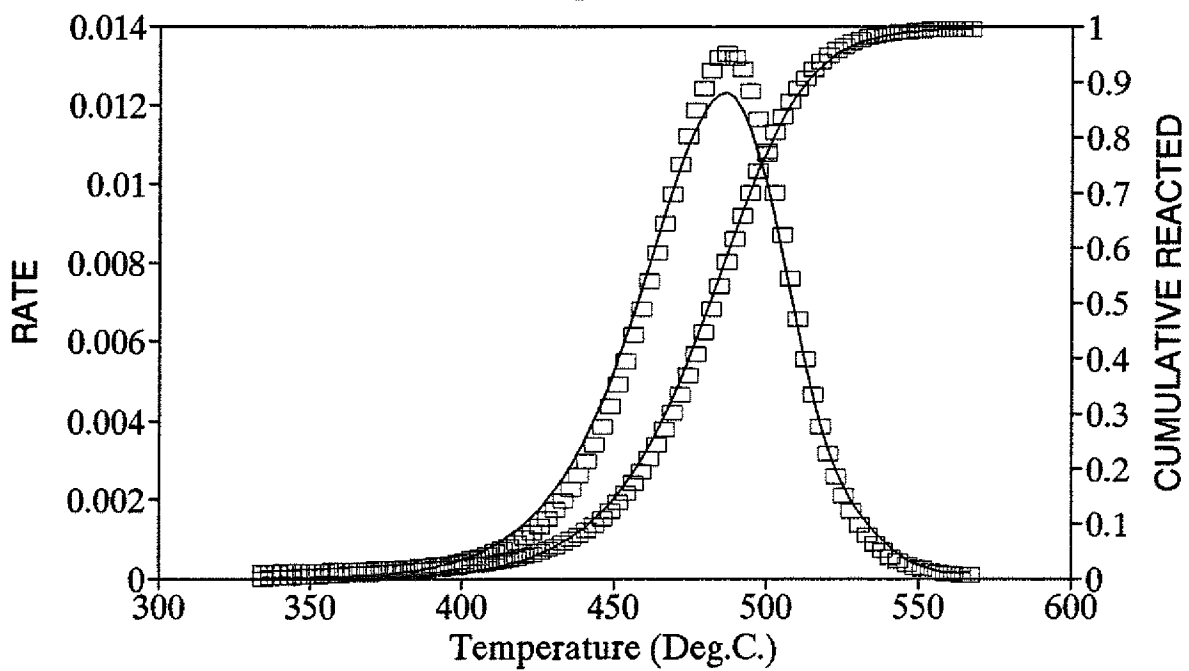


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EXPERIMENTAL & COMPUTED PYROGRAMS

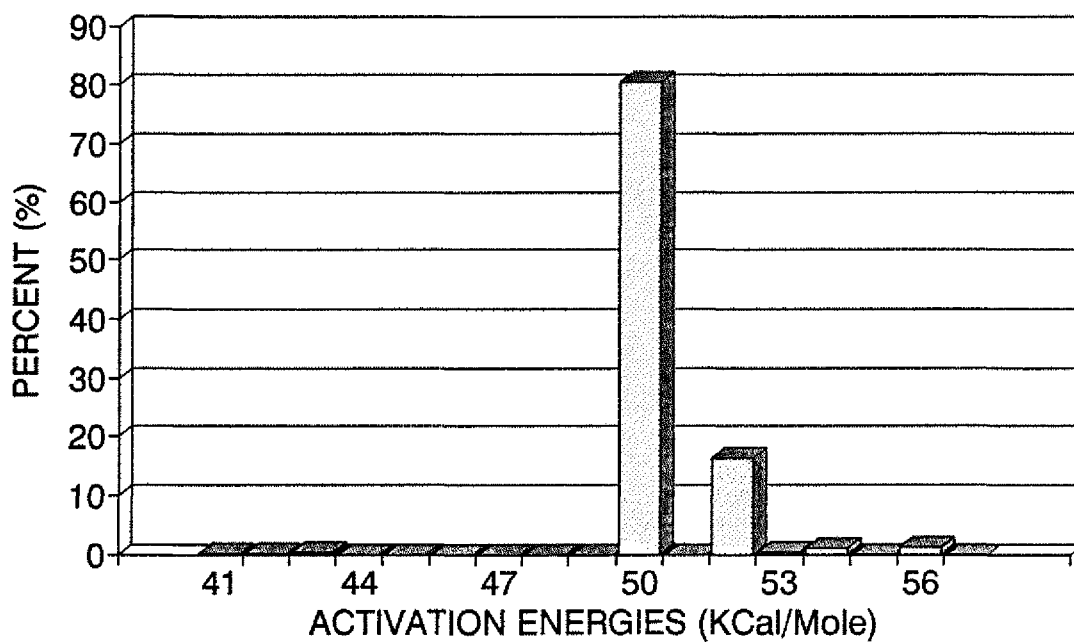
Sample 362



□ c:\kinetics\stat01\36250.prn — COMPUTED

ACTIVATION ENERGIES DISTRIBUTION

Sample 363



Frequency factor = $7.6403E+12 \text{ s}^{-1}$

Sample 363

Fitting method: Discrete (option 1)
Least squares of: Relative Rates
Error tolerance for initial search: 1.0000E-01
Error tolerance for final convergence: 1.0000E-02
Thermal history: Constant heating rate (max. rel. std. dev. =

Initial minimum frequency factor(s⁻¹): 1.4987E+11
Initial maximum frequency factor(s⁻¹): 1.4987E+13

Results

Frequency factor = 7.6403E+12 s⁻¹

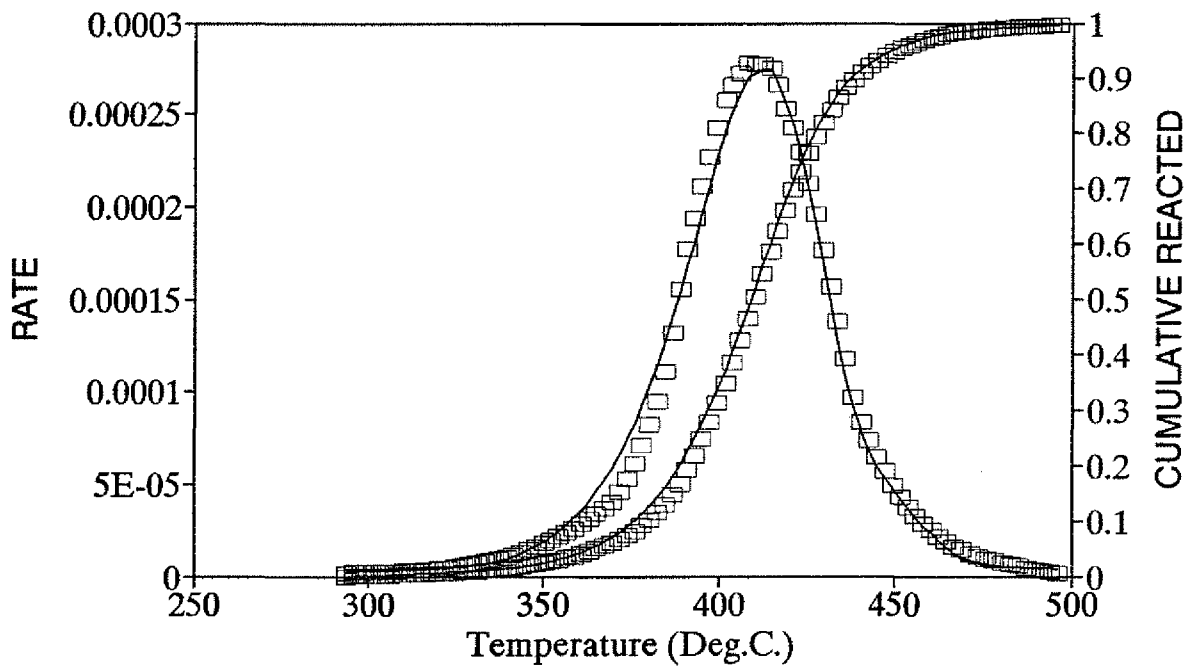
Percent	Activation energy (cal/mol)
.07	41000.
.11	42000.
.42	43000.
.00	44000.
.00	45000.
.00	46000.
.00	47000.
.00	48000.
.00	49000.
80.40	50000.
.00	51000.
16.42	52000.
.36	53000.
.92	54000.
.00	55000.
1.30	56000.

Least squares exit: successful completion

Sum of squares of weighted normalized rate residuals: 2.0000E-01
Sum of squares of weighted integrated rate residuals: 3.1594E-02

EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 363

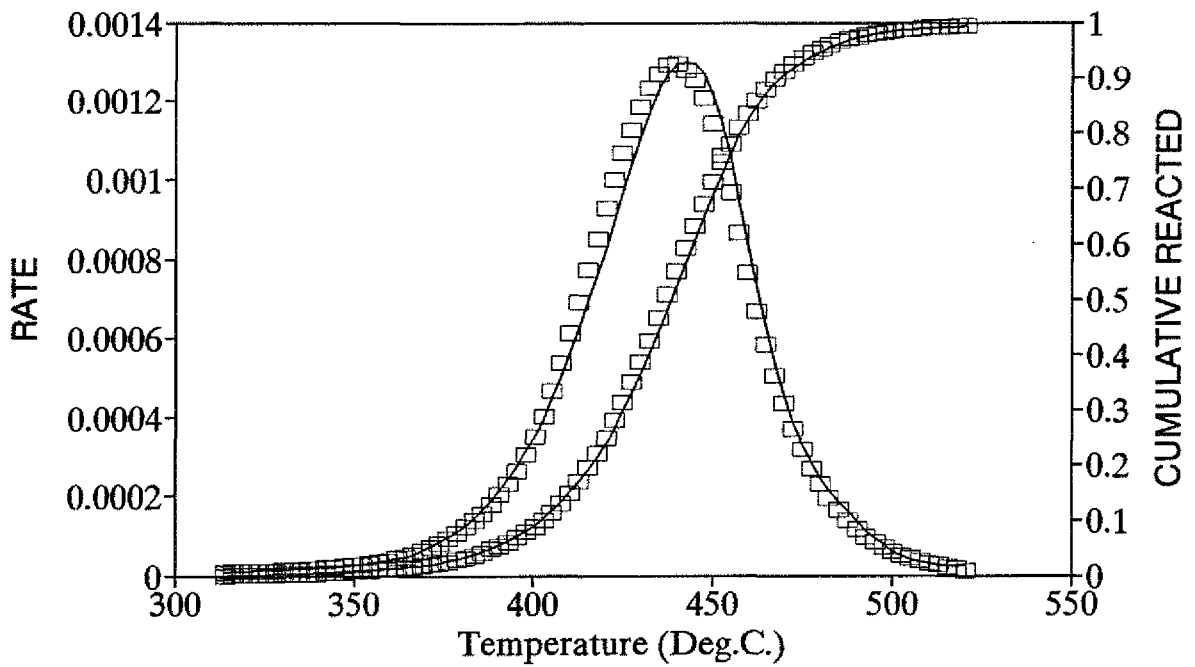


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— COMPUTED

EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 363

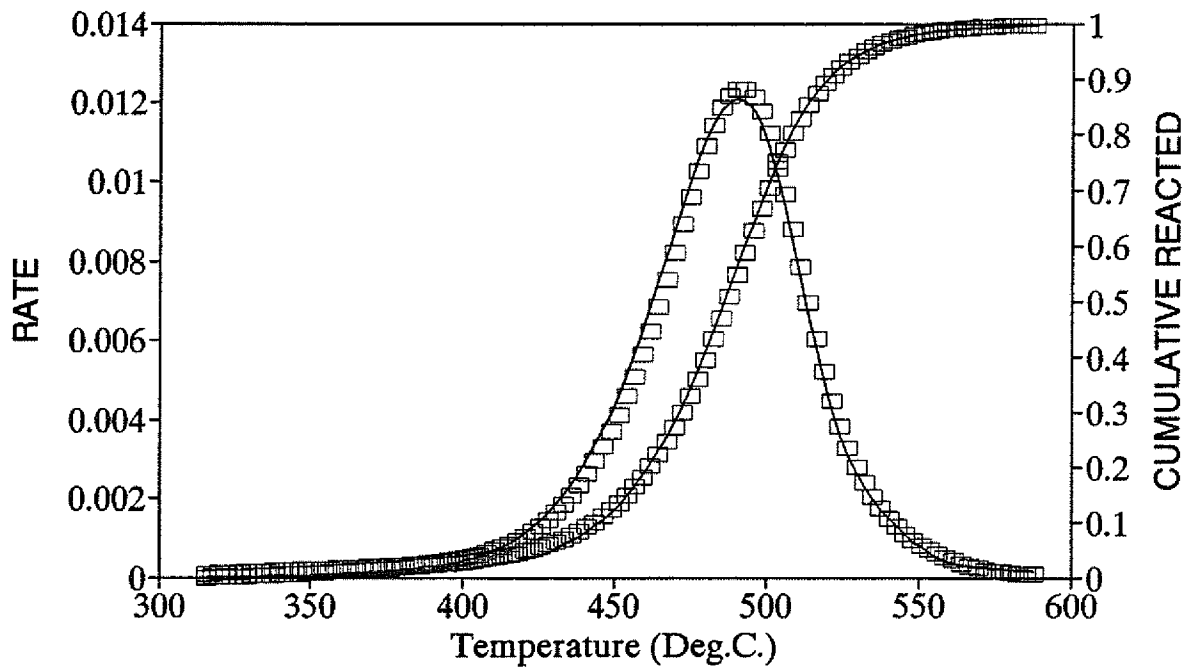


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EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 363

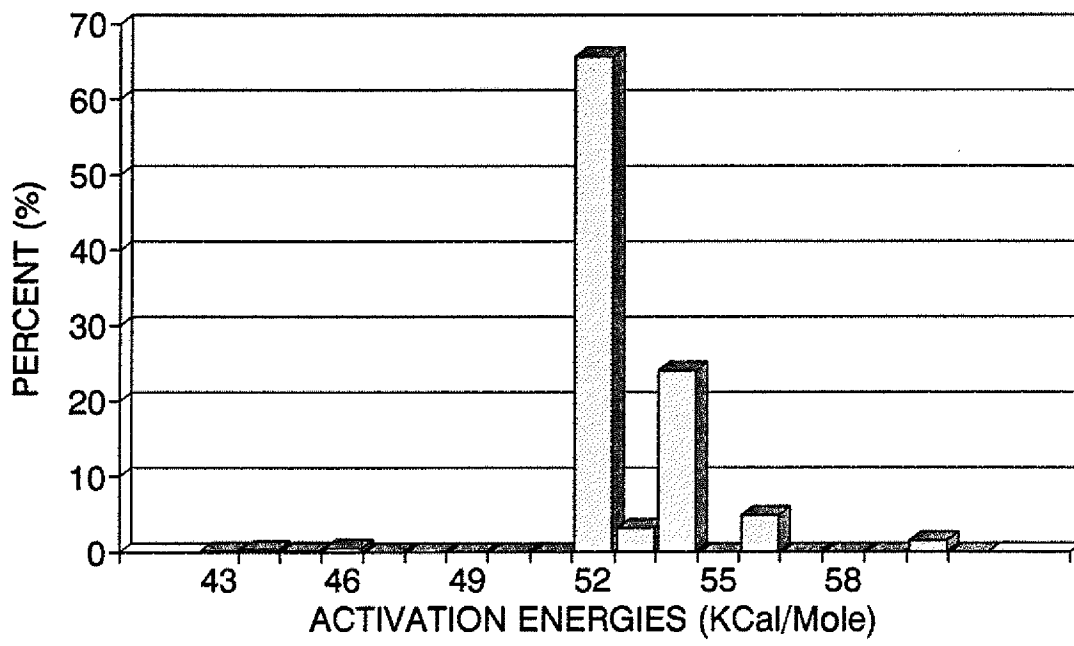


□ c:\kinetics\stat01\36350.prn

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ACTIVATION ENERGIES DISTRIBUTION

Sample 364



Frequency factor = $5.0215E+13 \text{ s}^{-1}$

Sample 364

Fitting method: Discrete (option 1)
Least squares of: Relative Rates
Error tolerance for initial search: 1.0000E-01
Error tolerance for final convergence: 1.0000E-02
Thermal history: Constant heating rate (max. rel. std. dev. =

Initial minimum frequency factor(s⁻¹): 1.1248E+12
Initial maximum frequency factor(s⁻¹): 1.1248E+14

Results

Frequency factor = 5.0215E+13 s⁻¹

Percent	Activation energy (cal/mol)
.05	43000.
.19	44000.
.09	45000.
.44	46000.
.00	47000.
.00	48000.
.00	49000.
.00	50000.
.00	51000.
65.70	52000.
3.19	53000.
24.16	54000.
.00	55000.
4.80	56000.
.00	57000.
.00	58000.
.00	59000.
1.39	60000.

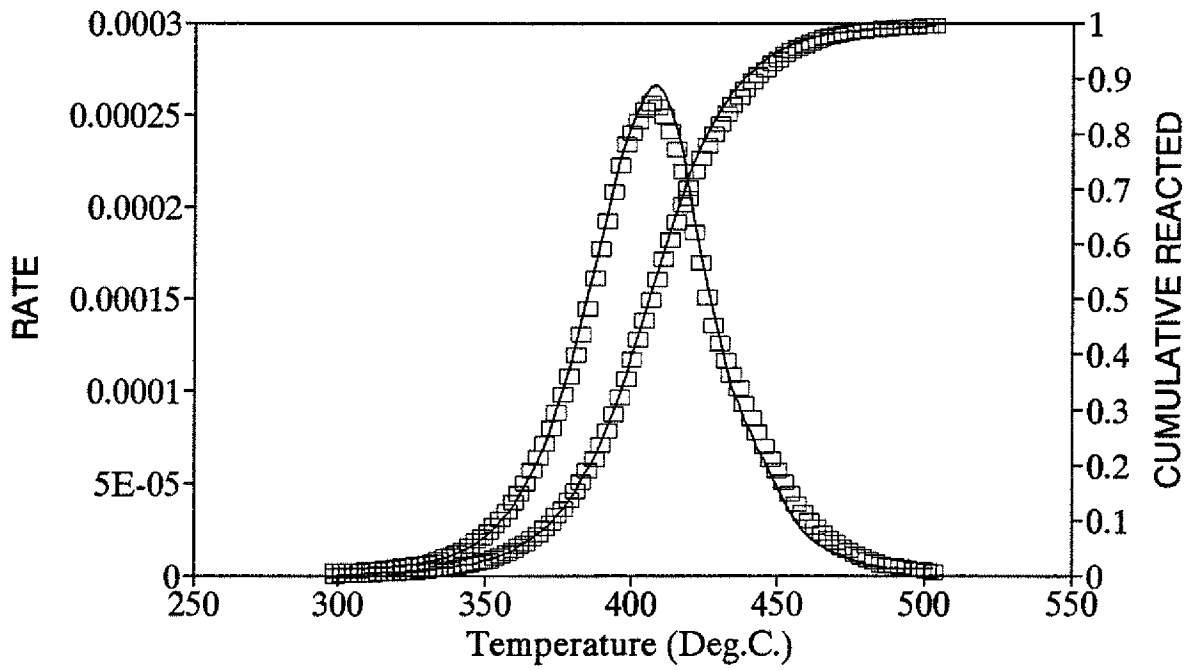
Least squares exit: successful completion

Sum of squares of weighted normalized rate residuals: 1.5290E-01

Sum of squares of weighted integrated rate residuals: 2.6156E-02

EXPERIMENTAL & COMPUTED PYROGRAMS

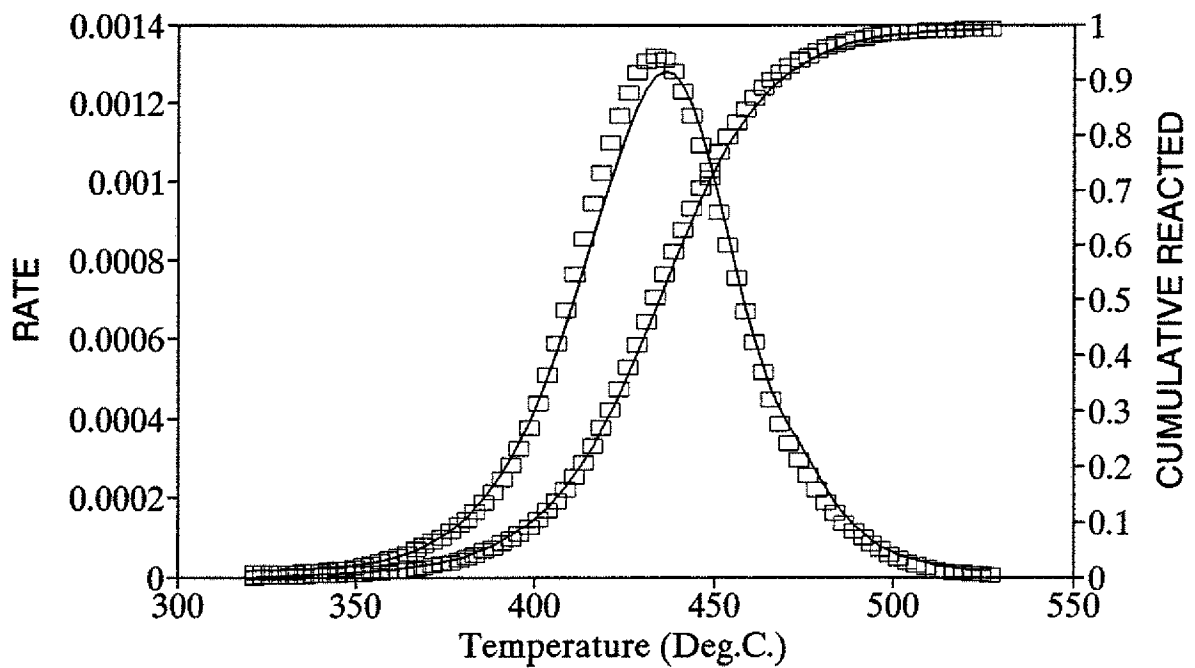
Sample 364



□ c:\kinetics\stat01\36401.prn — COMPUTED

EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 364

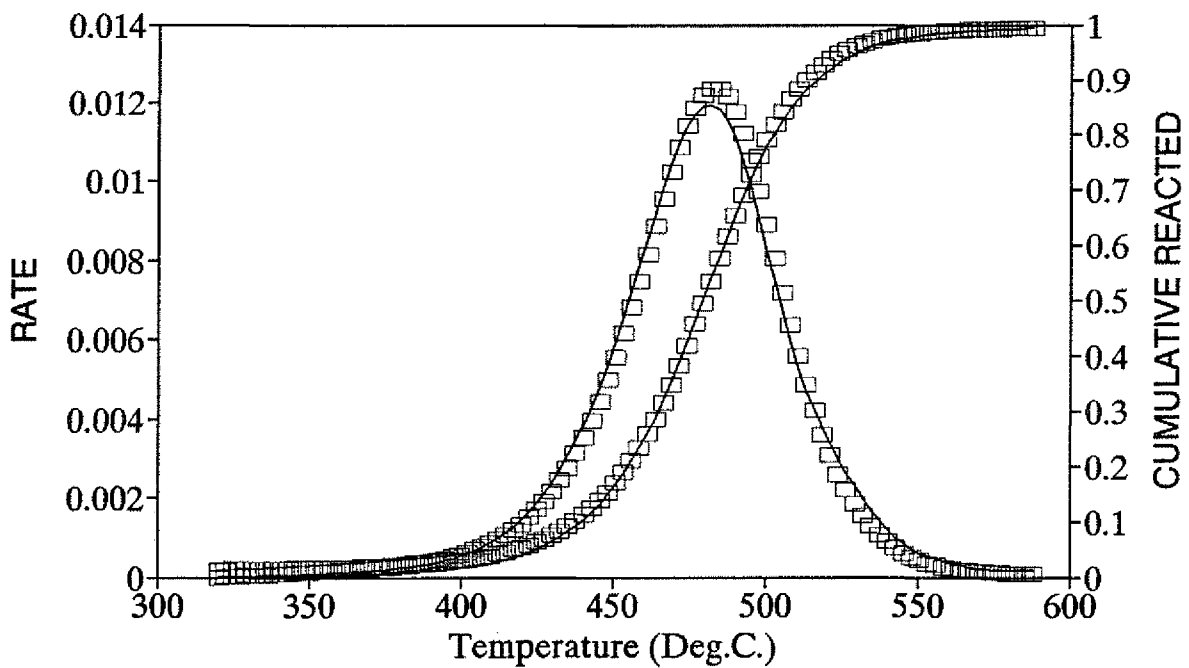


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EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 364

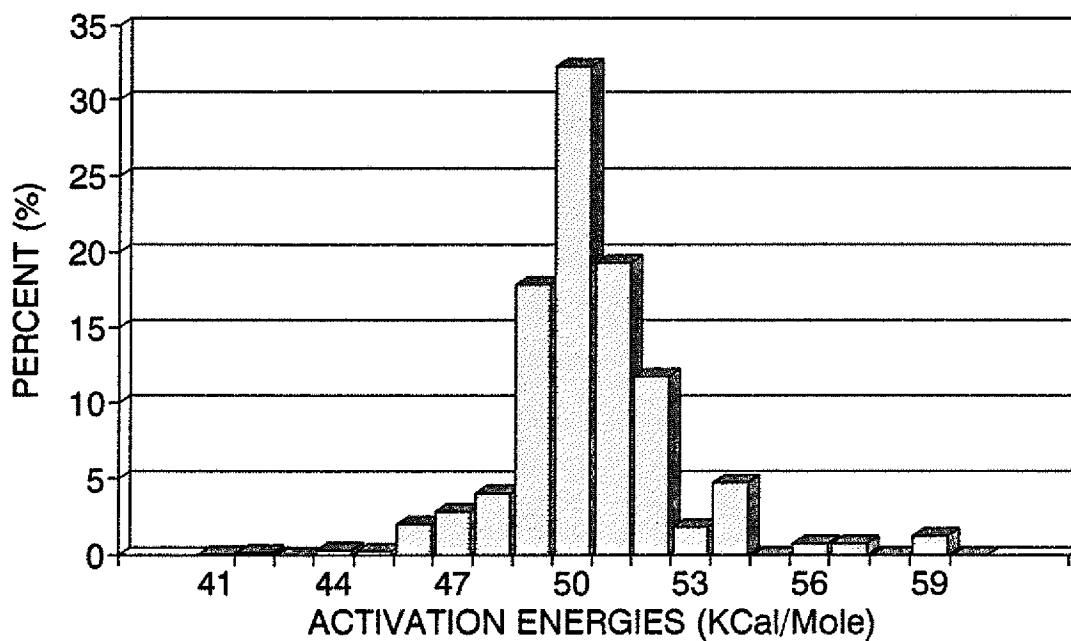


□ c:\kinetics\stat01\36450.prn

— COMPUTED

ACTIVATION ENERGIES DISTRIBUTION

Sample 365



Frequency factor = $9.7710E+12 \text{ s}^{-1}$

Sample 365

Fitting method: Discrete (option 1)
Least squares of: Relative Rates
Error tolerance for initial search: 1.0000E-01
Error tolerance for final convergence: 1.0000E-02
Thermal history: Constant heating rate (max. rel. std. dev. =

Initial minimum frequency factor(s⁻¹): 7.1068E+11
Initial maximum frequency factor(s⁻¹): 7.1068E+13

Results

Frequency factor = 9.7710E+12 s⁻¹

Percent	Activation energy (cal/mol)
.05	41000.
.17	42000.
.00	43000.
.33	44000.
.19	45000.
2.04	46000.
2.82	47000.
4.04	48000.
17.87	49000.
32.24	50000.
19.25	51000.
11.78	52000.
1.83	53000.
4.70	54000.
.00	55000.
.75	56000.
.70	57000.
.00	58000.
1.26	59000.

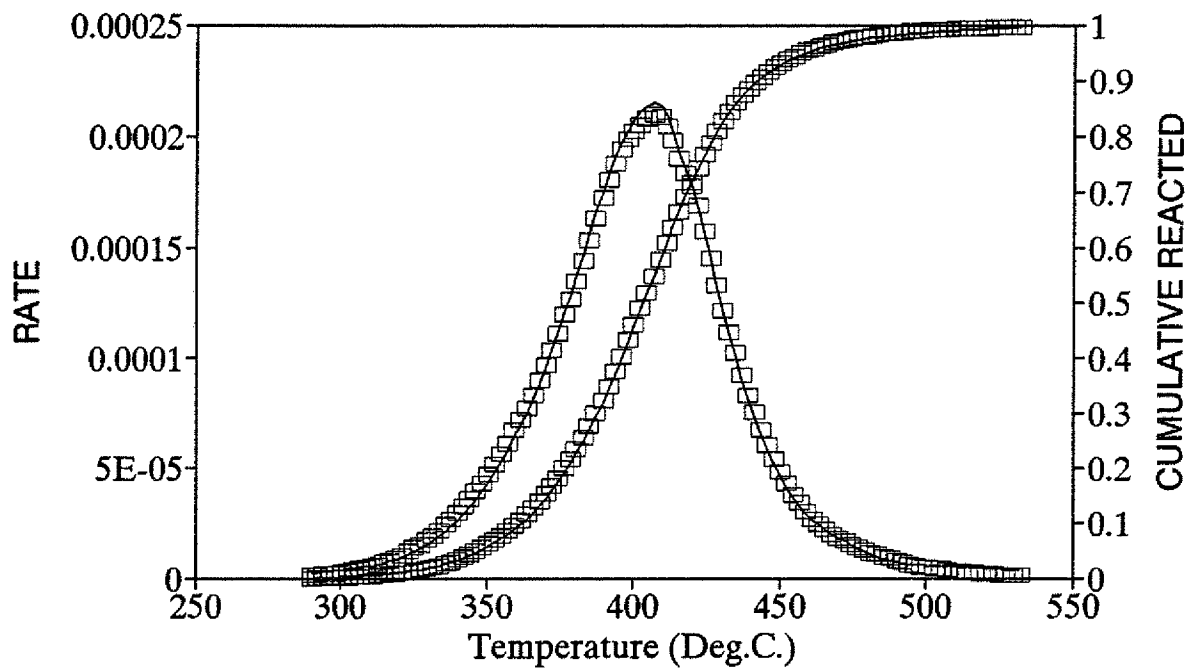
Least squares exit: successful completion

Sum of squares of weighted normalized rate residuals: 5.8294E-02

Sum of squares of weighted integrated rate residuals: 7.4633E-03

EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 365

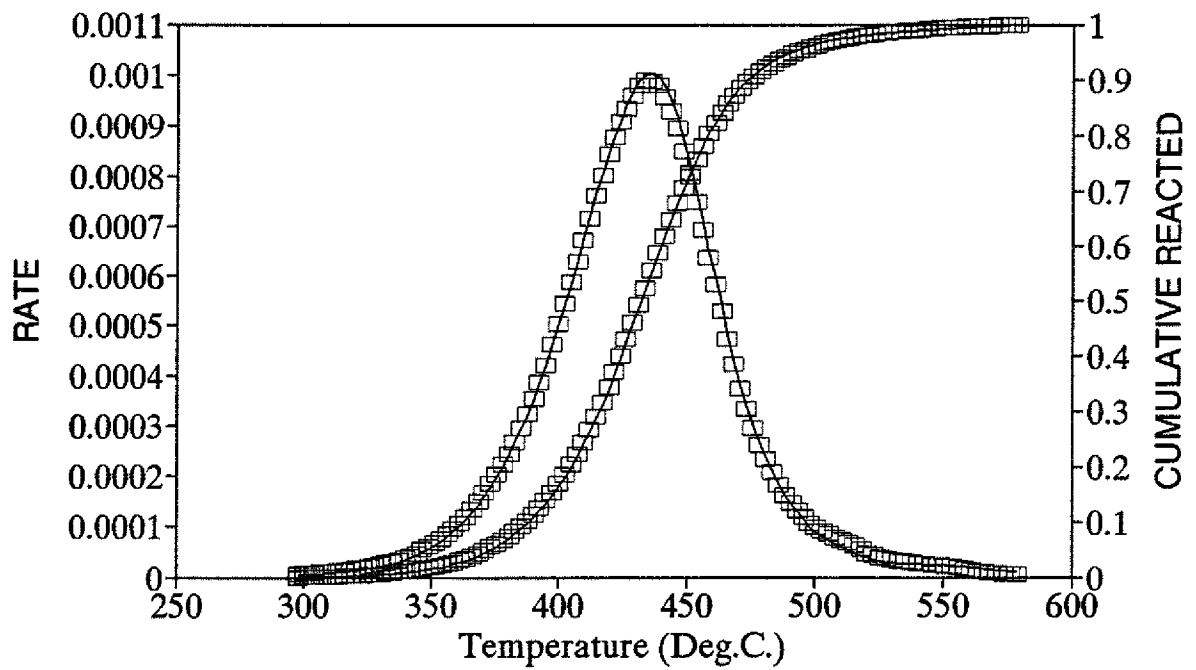


□ c:\kinetics\stat01\36501.prn

— COMPUTED

EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 365

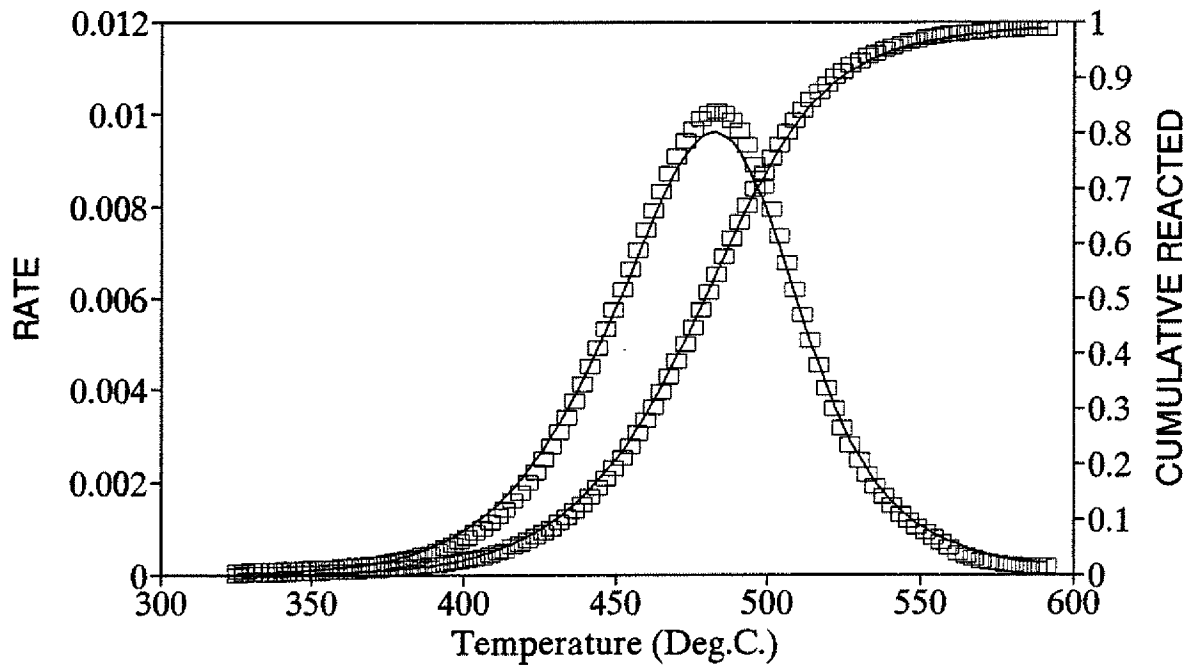


□ c:\kinetics\stat01\36505.prn

— COMPUTED

EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 365

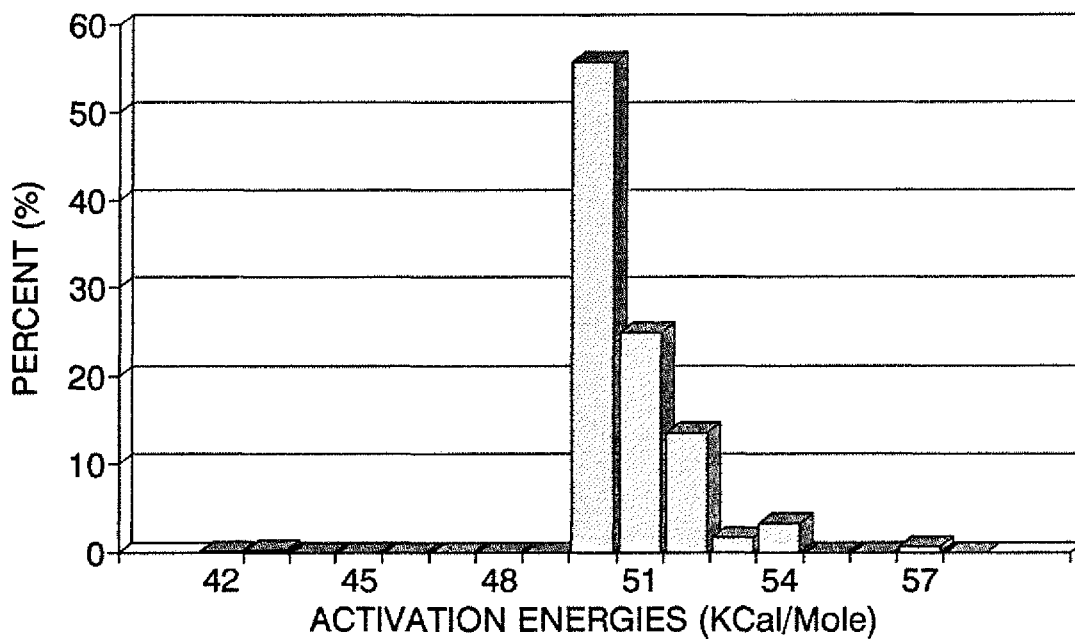


□ c:\kinetics\stat01\36550.prn

— COMPUTED

ACTIVATION ENERGIES DISTRIBUTION

Sample 366



Frequency factor = $1.0688E+13 \text{ s}^{-1}$

Sample 366

Fitting method: Discrete (option 1)
Least squares of: Relative Rates
Error tolerance for initial search: 1.0000E-01
Error tolerance for final convergence: 1.0000E-02
Thermal history: Constant heating rate (max. rel. std. dev. =

Initial minimum frequency factor(s^{-1}): 5.9090E+11
Initial maximum frequency factor(s^{-1}): 5.9090E+13

Results

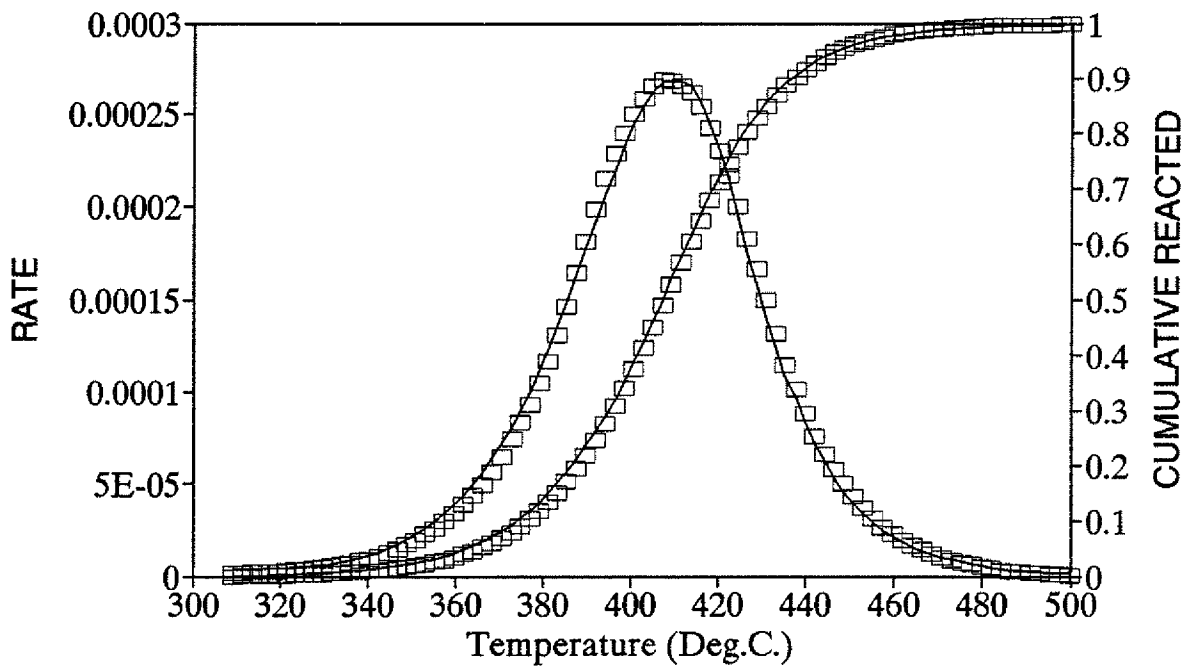
Frequency factor = 1.0688E+13 s^{-1}
Percent Activation energy (cal/mol)

.02	42000.
.24	43000.
.00	44000.
.00	45000.
.00	46000.
.00	47000.
.00	48000.
.00	49000.
55.75	50000.
24.82	51000.
13.55	52000.
1.68	53000.
3.32	54000.
.00	55000.
.00	56000.
.62	57000.

Least squares exit: successful completion
Sum of squares of weighted normalized rate residuals: 3.8772E-02
Sum of squares of weighted integrated rate residuals: 1.3684E-02

EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 366

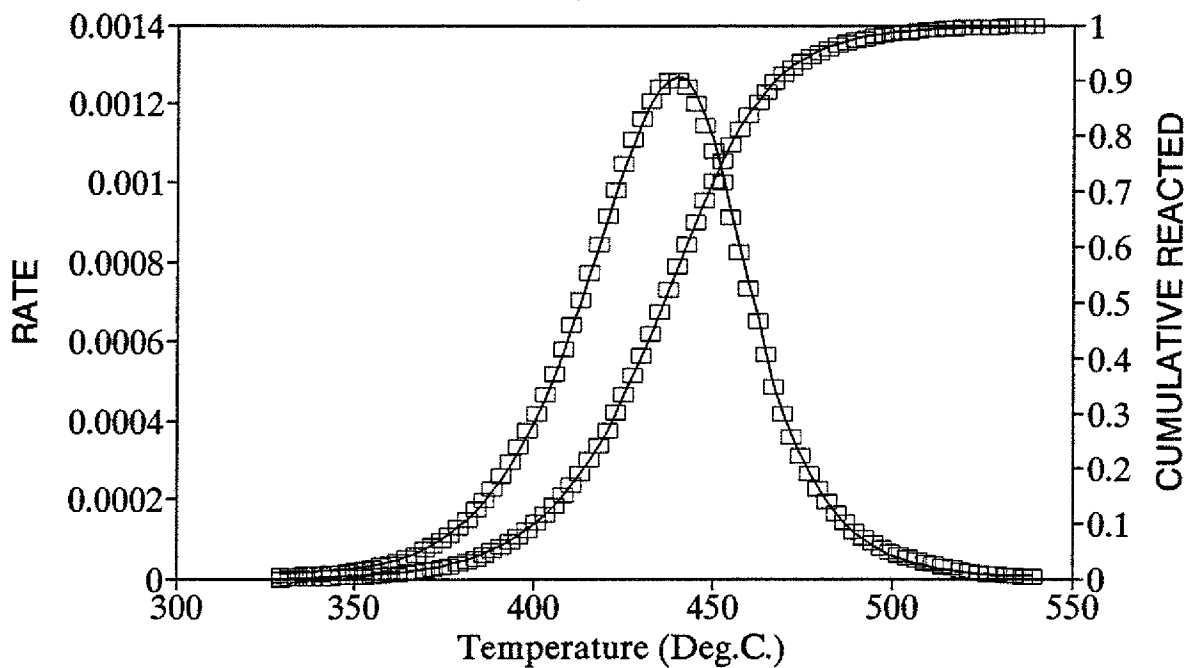


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— COMPUTED

EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 366

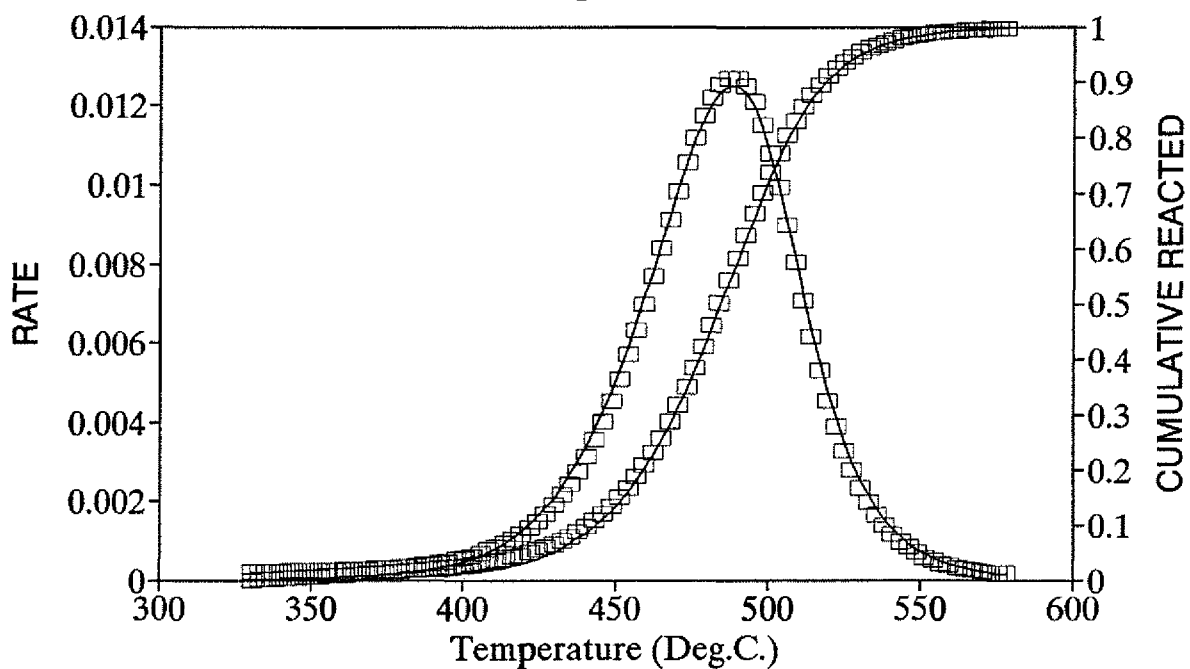


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— COMPUTED

EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 366

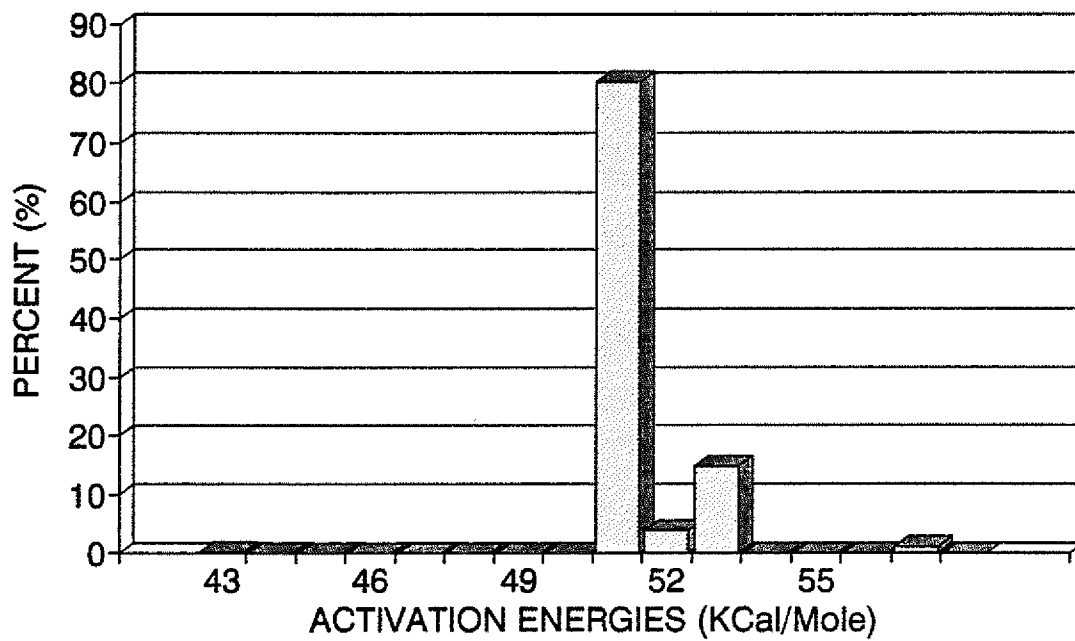


□ c:\kinetics\stat01\36650.prn

— COMPUTED

ACTIVATION ENERGIES DISTRIBUTION

Sample 367



Frequency factor = $1.9678E+13 \text{ s}^{-1}$

Sample 367

Fitting method: Discrete (option 1)
Least squares of: Relative Rates
Error tolerance for initial search: 1.0000E-01
Error tolerance for final convergence: 1.0000E-02
Thermal history: Constant heating rate (max. rel. std. dev. =

Initial minimum frequency factor(s⁻¹): 3.7778E+11
Initial maximum frequency factor(s⁻¹): 3.7778E+13

Results

Frequency factor = 1.9678E+13 s⁻¹

Percent	Activation energy (cal/mol)
.11	43000.
.00	44000.
.00	45000.
.00	46000.
.00	47000.
.00	48000.
.00	49000.
.00	50000.
80.28	51000.
3.74	52000.
14.89	53000.
.00	54000.
.00	55000.
.00	56000.
.97	57000.

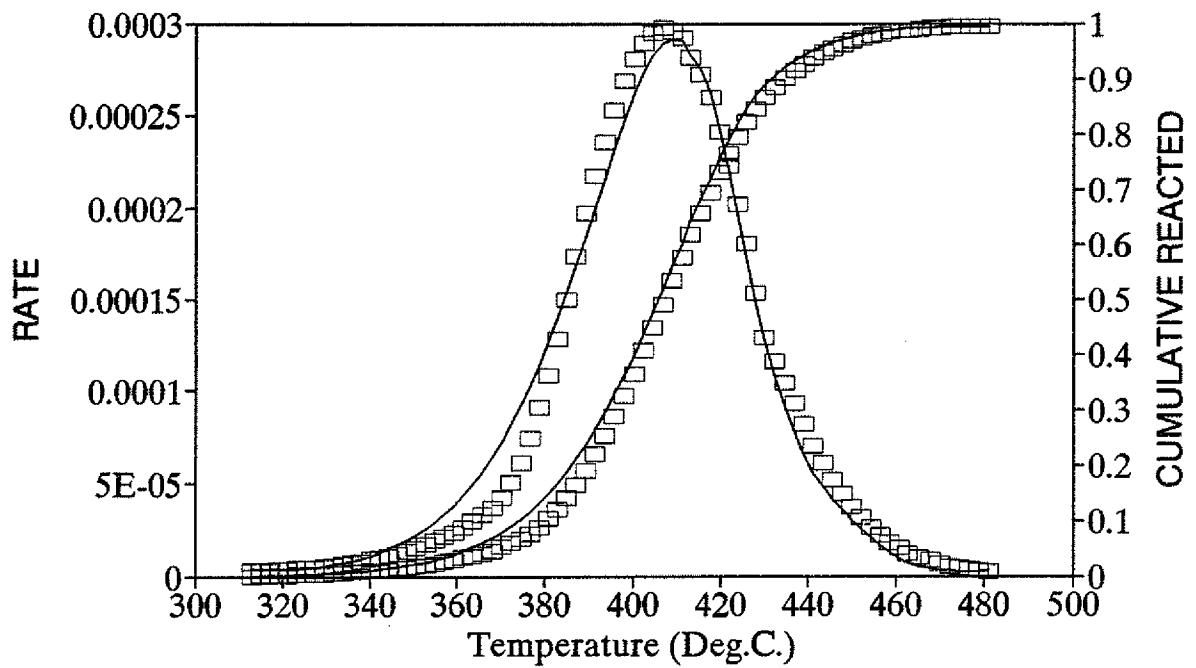
Least squares exit: successful completion

Sum of squares of weighted normalized rate residuals: 2.5631E-01

Sum of squares of weighted integrated rate residuals: 5.5659E-02

EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 367

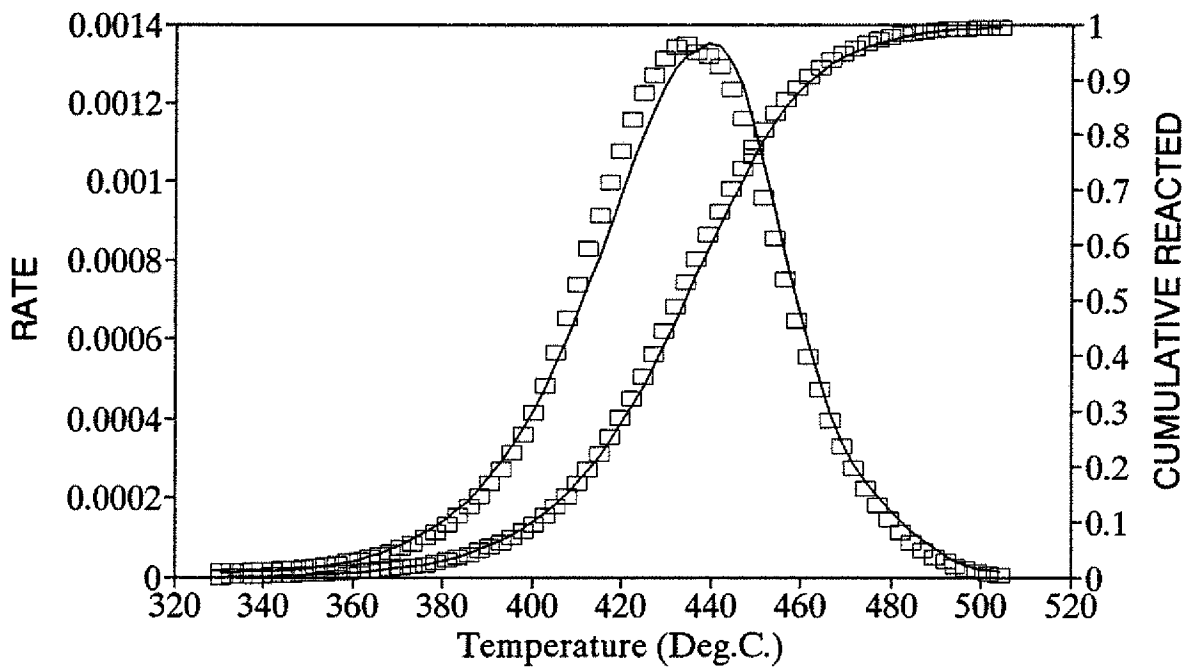


□ c:\kinetics\stat01\36701.prn

— COMPUTED

EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 367

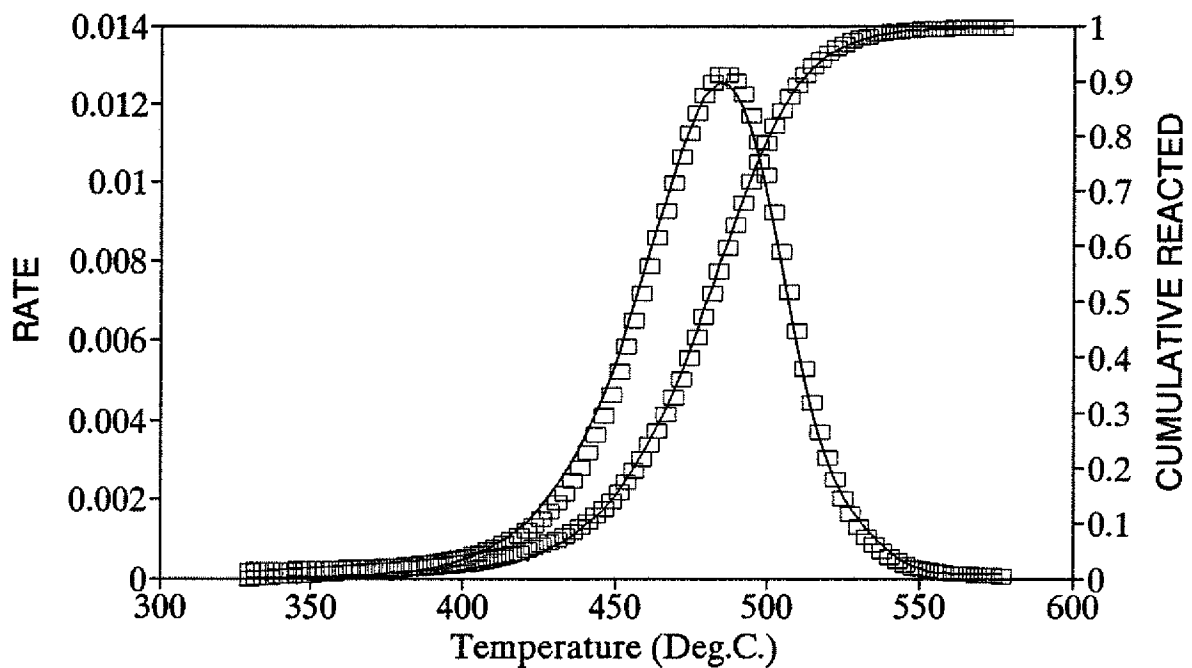


□ c:\kinetics\stat01\36705.prn

— COMPUTED

EXPERIMENTAL & COMPUTED PYROGRAMS

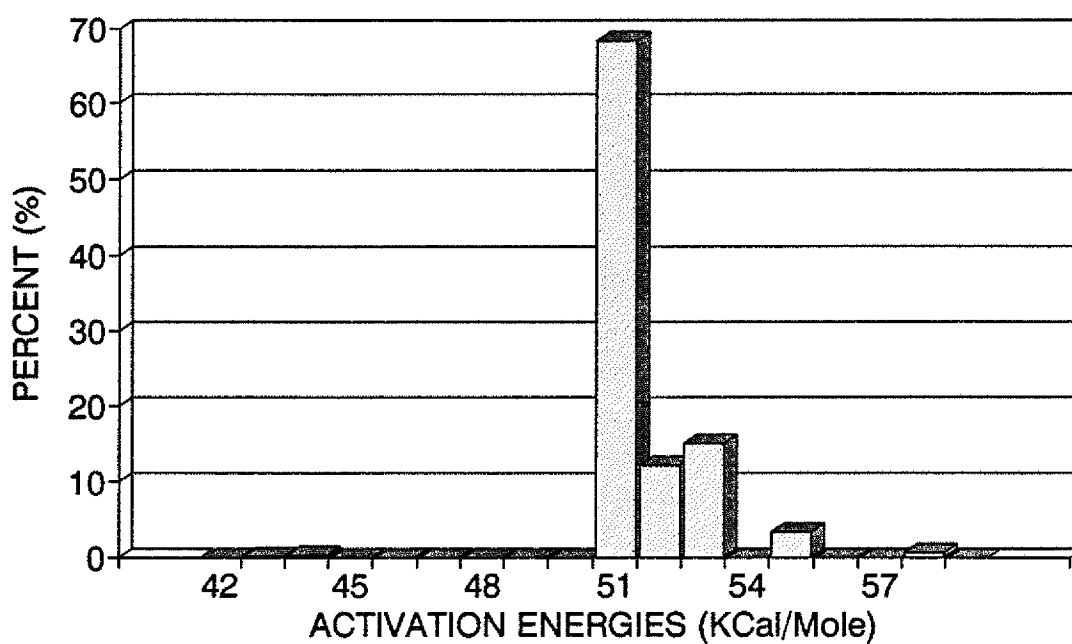
Sample 367



□ c:\kinetics\stat01\36750b.prn — COMPUTED

ACTIVATION ENERGIES DISTRIBUTION

Sample 368



Frequency factor = $1.7543E+13 \text{ s}^{-1}$

Sample 368

Fitting method: Discrete (option 1)
Least squares of: Relative Rates
Error tolerance for initial search: 1.0000E-01
Error tolerance for final convergence: 1.0000E-02
Thermal history: Constant heating rate (max. rel. std. dev. =

Initial minimum frequency factor(s⁻¹): 7.0318E+11
Initial maximum frequency factor(s⁻¹): 7.0318E+13

Results

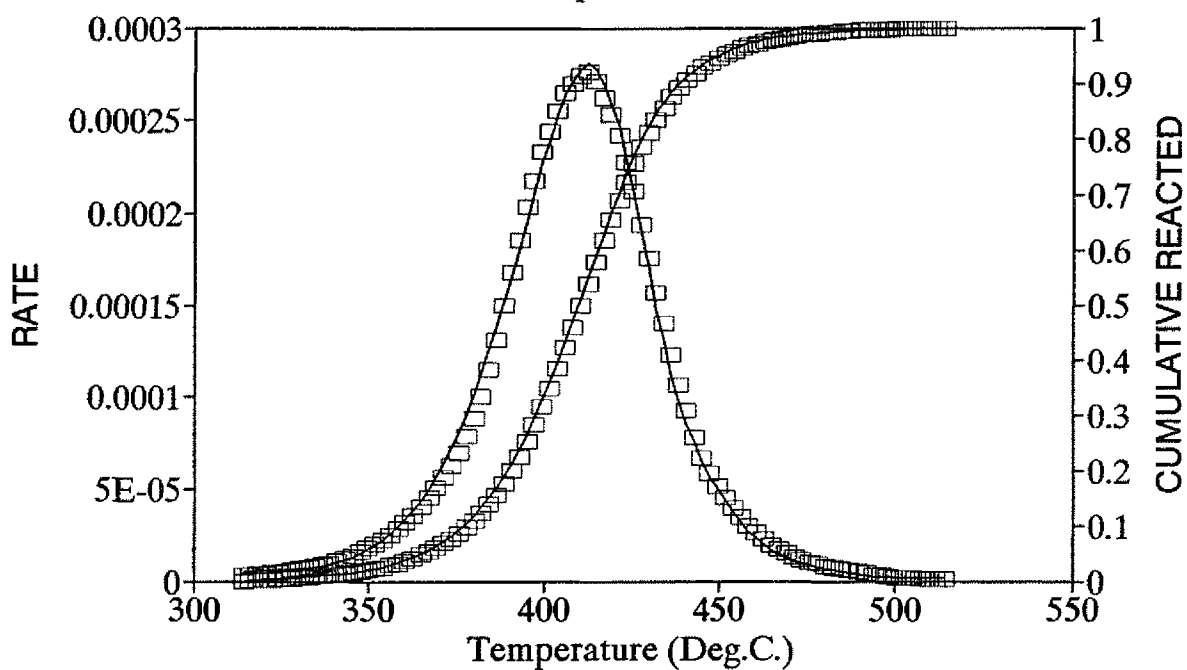
Frequency factor = 1.7543E+13 s⁻¹

Percent	Activation energy (cal/mol)
.00	42000.
.10	43000.
.32	44000.
.00	45000.
.00	46000.
.00	47000.
.00	48000.
.00	49000.
.00	50000.
68.45	51000.
12.14	52000.
15.06	53000.
.00	54000.
3.30	55000.
.00	56000.
.00	57000.
.62	58000.

Least squares exit: successful completion
Sum of squares of weighted normalized rate residuals: 1.2281E-01
Sum of squares of weighted integrated rate residuals: 1.7951E-02

EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 368

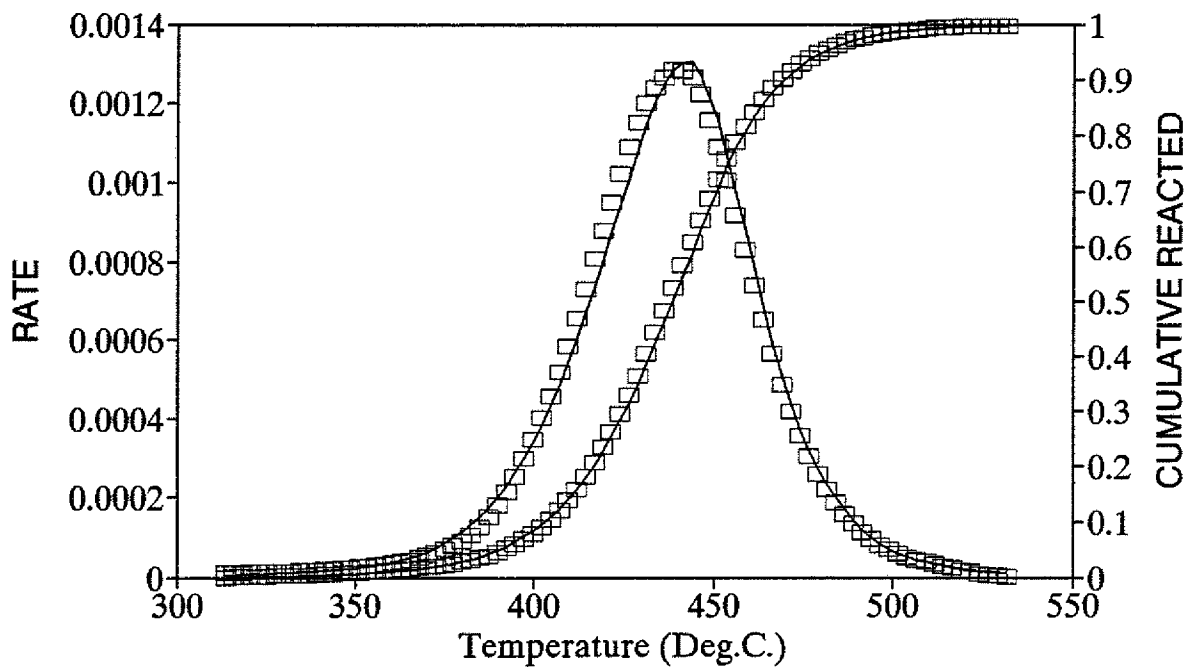


□ c:\kinetics\stat01\36801.prm

— COMPUTED

EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 368

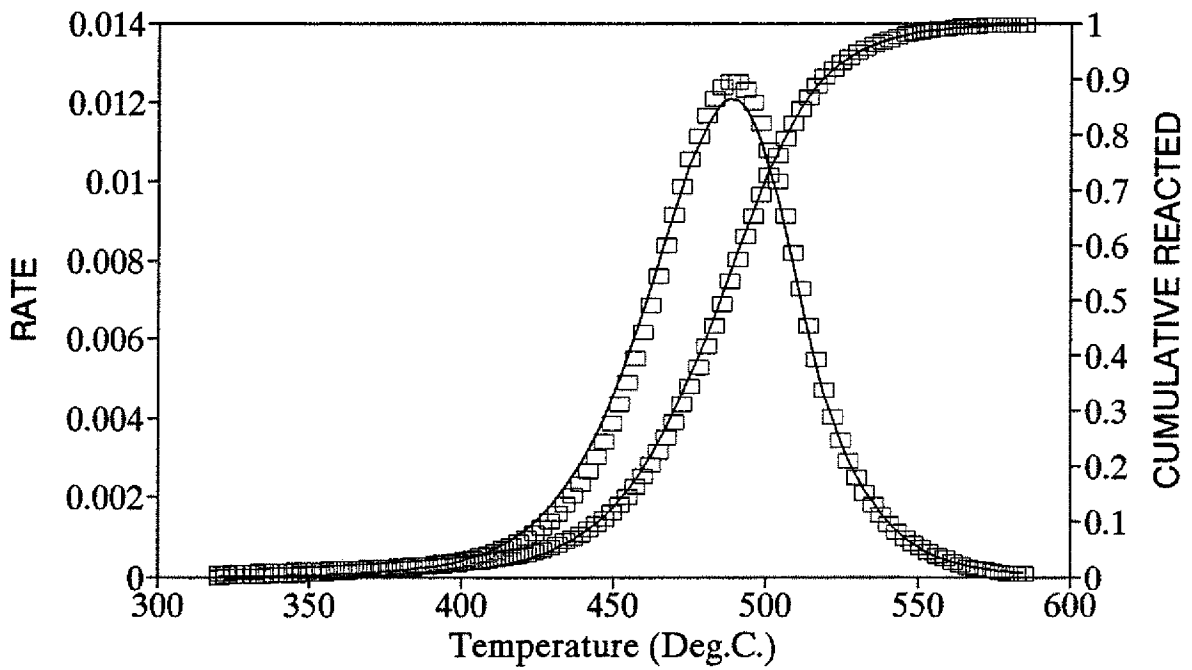


□ c:\kinetics\stat01\36805.prn

— COMPUTED

EXPERIMENTAL & COMPUTED PYROGRAMS

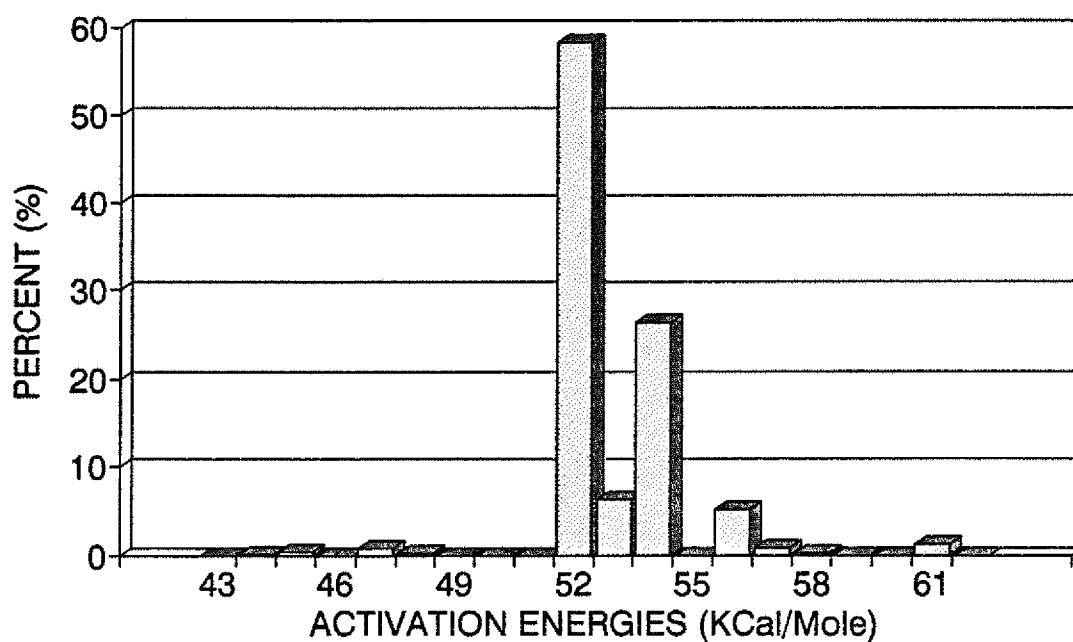
Sample 368



□ c:\kinetics\stat01\36850.prn — COMPUTED

ACTIVATION ENERGIES DISTRIBUTION

Sample 369



Frequency factor = $5.5349E+13 \text{ s}^{-1}$

Sample 369

Fitting method: Discrete (option 1)
Least squares of: Relative Rates
Error tolerance for initial search: 1.0000E-01
Error tolerance for final convergence: 1.0000E-02
Thermal history: Constant heating rate (max. rel. std. dev. =

Initial minimum frequency factor(s⁻¹): 6.2547E+11
Initial maximum frequency factor(s⁻¹): 6.2547E+13

Results

Frequency factor = 5.5349E+13 s⁻¹
Percent Activation energy (cal/mol)

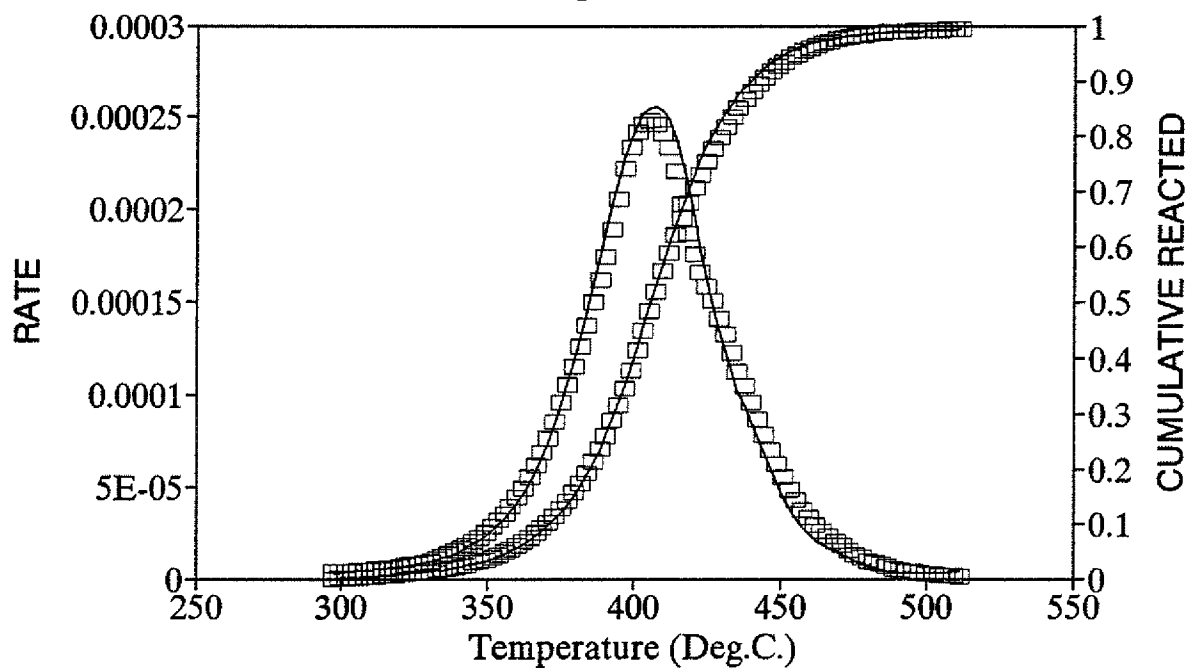
.00	43000.
.08	44000.
.43	45000.
.00	46000.
.77	47000.
.26	48000.
.00	49000.
.00	50000.
.00	51000.
58.33	52000.
6.33	53000.
26.37	54000.
.00	55000.
5.23	56000.
.75	57000.
.15	58000.
.00	59000.
.00	60000.
1.29	61000.

Least squares exit: successful completion

Sum of squares of weighted normalized rate residuals: 2.3657E-01
Sum of squares of weighted integrated rate residuals: 4.3515E-02

EXPERIMENTAL & COMPUTED PYROGRAMS

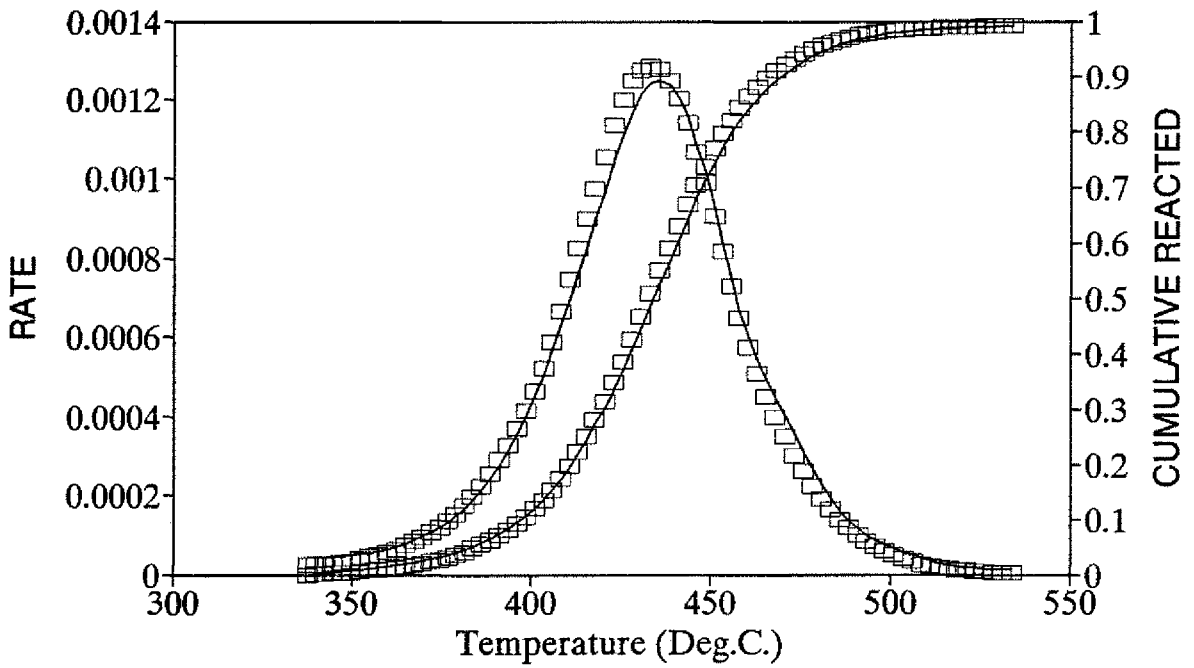
Sample 369



□ c:\kinetics\stat01\36901.prn — COMPUTED

EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 369

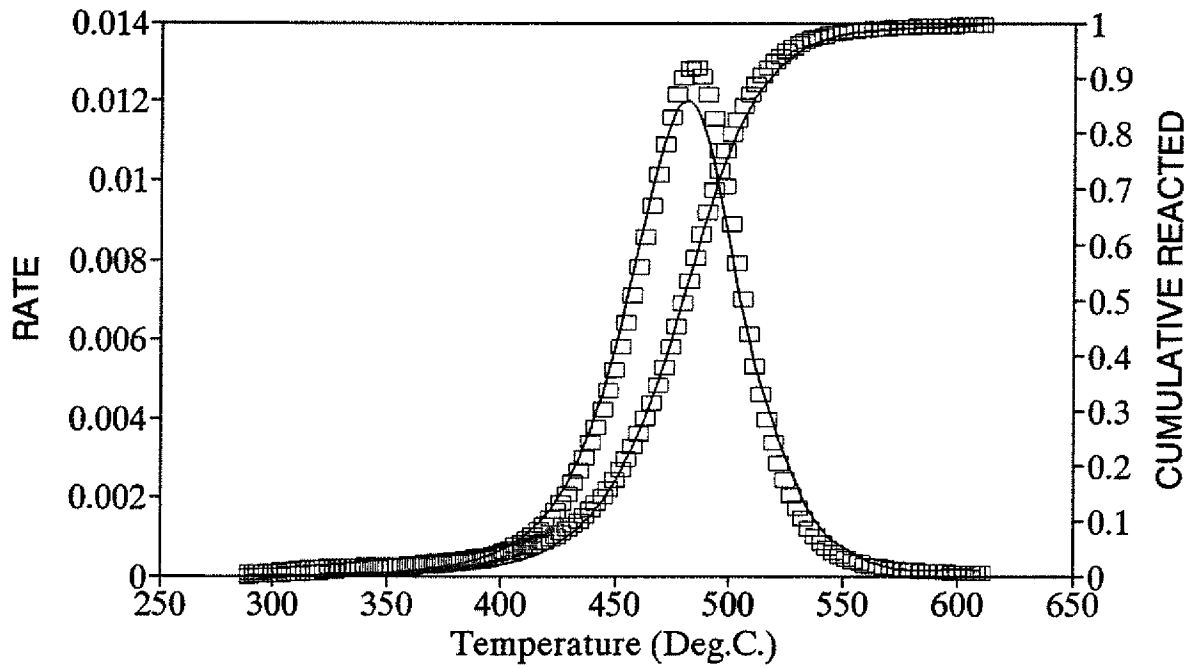


□ c:\kinetics\stat01\36905.prn

— COMPUTED

EXPERIMENTAL & COMPUTED PYROGRAMS

Sample 369



□ c:\kinetics\stat01\36950.prn

— COMPUTED

Sample 361

Code Version: 2.43

Output File: c:\kinetics\stat01\361.out

Data file	Number of data		Group
	(total)	(used)	weight
c:\kinetics\stat01\36101.prn	84	84	1.0000E+00
c:\kinetics\stat01\36105.prn	78	78	1.0000E+00
c:\kinetics\stat01\36150.prn	97	97	1.0000E+00

Title line of data files:

W=40 N=3 -1.3 C/Hr. MaxFid= 4395E-1 Int =16288668E-1 Sample 361

W=21 N=3 4.6 C/Mn. MaxFid= 1017E-0 Int =799013E-0 Sample 361

W=14 N=3 43.0 C/Mn. MaxFid= 8816E-0 Int =713201E-0 sample 361

Friedman-type analysis at fraction reacted = x

(Valid only if data extend to nearly complete reaction)

x	$\ln[A(1-x)^n]$	A (for n=1) (s ⁻¹)	E (cal/mol)	E std.err. (cal/mol)
.1	2.9245E+01	5.582E+12	49603.	2987.
.2	3.0062E+01	1.421E+13	50938.	2000.
.3	2.9812E+01	1.266E+13	50819.	710.
.4	2.9858E+01	1.546E+13	51154.	535.
.5	3.0059E+01	2.267E+13	51778.	657.
.6	3.0299E+01	3.603E+13	52561.	805.
.7	3.0429E+01	5.472E+13	53345.	953.
.8	3.0384E+01	7.847E+13	54154.	1115.
.9	3.1119E+01	3.271E+14	56897.	2154.

Mean approximate A and E over fraction-reacted interval from 0 to x

(Valid only if data extend to nearly complete reaction)

x	A (s ⁻¹)	E (cal/mol)	E std.err. (cal/mol)
.1	3.1854E+14	50844.	1964.
.2	8.5494E+13	50606.	2404.
.3	4.2030E+13	50706.	2194.
.4	2.2858E+13	50771.	1661.
.5	1.5064E+13	51045.	1283.
.6	9.9727E+12	51335.	1065.
.7	6.6473E+12	51731.	895.
.8	4.9287E+12	52515.	1013.
.9	3.2015E+12	53765.	1336.

Interpolation from parabolic fit of Tmax vs. log(Heating rate):

Tmax = 472.90 C at Heating rate = 25 C/min

Interpolation from linear fit of FWHH vs. log(Heating rate):

FWHH = 55.22 C at Heating rate = 25 C/min

Interpolation from linear fit of Asymmetry vs. log(Heating rate):

Asymmetry = .786 at Heating rate = 25 C/min

Approximate fit of disk data to a single first-order reaction:

Data	Heating rate	Tmax	Exp.FWHH	Cal.FWHH	Exp./Calc.
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Asymmetry

	(C/min)	(C)	(C)	(C)	
1	9.0332E-01	408.93	47.88	43.95	1.08941
.9064					
2	4.5843E+00	439.06	53.85	47.82	1.12614
.7821					
3	4.6968E+01	486.47	55.65	54.30	1.02484
.7900					

A(s⁻¹) = 6.8318E+12
 E(cal/mol) = 4.9798E+04 (std. err. = 1.540E+02)
 S(%E) = 1.0871E+00
 n(order) = 1.0000e+00

Fitting method: Discrete (option 1)
 Least squares of: Relative Rates
 Error tolerance for initial search: 1.0000E-01
 Error tolerance for final convergence: 1.0000E-02
 Thermal history: Constant heating rate (max. rel. std. dev. = 7.878E-04)

Initial minimum frequency factor(s⁻¹): 6.8318E+11
 Initial maximum frequency factor(s⁻¹): 6.8318E+13

Results

Frequency factor = 1.7717E+13 s⁻¹
 Percent Activation energy (cal/mol)

.09	43000.
.10	44000.
.00	45000.
.00	46000.
.07	47000.
.00	48000.
.00	49000.
8.85	50000.
63.51	51000.
9.58	52000.
15.30	53000.
.00	54000.
2.23	55000.
.00	56000.
.28	57000.

Least squares exit: successful completion
 Sum of squares of weighted normalized rate residuals: 6.0275E-02
 Sum of squares of weighted integrated rate residuals: 1.2208E-02

Time(s)	Temp(C)	Exp.Rate	Calc.Rate	Exp.Cum.
Calc.Cum.				

Data file: c:\kinetics\stat01\36101.prn
 SFACT = 3.7089E+06, WTR = 3.6843E+03, WTI = 1.0000E+00

3.7440E+03	3.1398E+02	2.2136E-06	3.9762E-06	0.0000E+00
0.0000E+00				
3.8880E+03	3.1601E+02	2.6073E-06	4.0633E-06	3.4710E-04
5.7762E-04				
4.0320E+03	3.1807E+02	2.9847E-06	4.1724E-06	7.4973E-04

Sample 362

Code Version: 2.43

Output File: c:\kinetics\stat01\362.out

Data file	Number of data		Group
	(total)	(used)	weight
c:\kinetics\stat01\36201.prn	84	84	1.0000E+00
c:\kinetics\stat01\36205.prn	76	76	1.0000E+00
c:\kinetics\stat01\36250.prn	94	94	1.0000E+00

Title line of data files:

W=35 N=3 -1.2 C/Hr. MaxFid= 4248E-1 Int =15449458E-1 Sample 362

W=20 N=3 4.5 C/Mn. MaxFid= 1456E-0 Int =1065726E-0 Sample 362

W=10 N=3 43.1 C/Mn. MaxFid= 6722E-0 Int =500224E-0 Sample 362

Friedman-type analysis at fraction reacted = x

(Valid only if data extend to nearly complete reaction)

x	ln[A(1-x)^n]	A(for n=1) (s^-1)	E (cal/mol)	E std.err. (cal/mol)
.1	2.8309E+01	2.190E+12	48407.	499.
.2	2.8603E+01	3.304E+12	48835.	1581.
.3	2.8767E+01	4.448E+12	49221.	1540.
.4	2.9181E+01	7.850E+12	50033.	1531.
.5	2.9604E+01	1.438E+13	50937.	1488.
.6	2.9979E+01	2.616E+13	51878.	1561.
.7	3.0459E+01	5.640E+13	53126.	1630.
.8	3.0903E+01	1.318E+14	54600.	1875.
.9	3.1733E+01	6.047E+14	57341.	3022.

Mean approximate A and E over fraction-reacted interval from 0 to x

(Valid only if data extend to nearly complete reaction)

x	A (s^-1)	E (cal/mol)	E std.err. (cal/mol)
.1	1.5327E+14	49933.	192.
.2	3.1437E+13	49283.	671.
.3	1.4248E+13	49203.	1180.
.4	8.0819E+12	49267.	1298.
.5	5.6344E+12	49571.	1381.
.6	4.2838E+12	50023.	1528.
.7	3.4297E+12	50639.	1465.
.8	3.0427E+12	51639.	1370.
.9	3.2865E+12	53547.	1886.

Interpolation from parabolic fit of Tmax vs. log(Heating rate):

Tmax = 472.29 C at Heating rate = 25 C/min

Interpolation from linear fit of FWHH vs. log(Heating rate):

FWHH = 51.07 C at Heating rate = 25 C/min

Interpolation from linear fit of Asymmetry vs. log(Heating rate):

Asymmetry = .756 at Heating rate = 25 C/min

Approximate fit of disk data to a single first-order reaction:

Data	Heating rate	Tmax	Exp.FWHH	Cal.FWHH	Exp./Calc.
------	--------------	------	----------	----------	------------

Asymmetry

	(C/min)	(C)	(C)	(C)	
1	9.0041E-01	407.15	47.15	45.09	1.04559
.9028					
2	4.5708E+00	435.95	49.90	49.18	1.01450
.8399					
3	4.7255E+01	486.95	51.49	56.10	.91790
.7238					

A(s⁻¹) = 2.1215E+12
 E(cal/mol) = 4.8014E+04 (std. err. = 1.396E+03)
 S(%E) = 4.1867E-01
 n(order) = 1.0000e+00

Fitting method: Discrete (option 1)
 Least squares of: Relative Rates
 Error tolerance for initial search: 1.0000E-01
 Error tolerance for final convergence: 1.0000E-02
 Thermal history: Constant heating rate (max. rel. std. dev. = 1.446E-03)

Initial minimum frequency factor(s⁻¹): 2.1215E+11
 Initial maximum frequency factor(s⁻¹): 2.1215E+13

Results

Frequency factor = 9.3831E+12 s⁻¹

Percent	Activation energy (cal/mol)
.05	42000.
.00	43000.
.00	44000.
.00	45000.
.00	46000.
.00	47000.
.00	48000.
.00	49000.
79.50	50000.
4.85	51000.
14.56	52000.
.00	53000.
.00	54000.
.00	55000.
1.05	56000.

Least squares exit: successful completion
 Sum of squares of weighted normalized rate residuals: 1.7182E-01
 Sum of squares of weighted integrated rate residuals: 2.0263E-02

Time(s)	Temp(C)	Exp.Rate	Calc.Rate	Exp.Cum.
Calc.Cum.				

Data file: c:\kinetics\stat01\36201.prn
 SFACT = 3.6471E+06, WTR = 3.6240E+03, WTI = 1.0000E+00

3.7440E+03	3.1334E+02	2.2511E-06	2.8034E-06	0.0000E+00
0.0000E+00				
3.8880E+03	3.1535E+02	2.4513E-06	2.9205E-06	3.3857E-04
4.1082E-04				
4.0320E+03	3.1736E+02	2.7200E-06	3.0843E-06	7.1090E-04

Sample 363

Code Version: 2.43

Output File: c:\kinetics\stat01\363.out

Data file	Number of data		Group
	(total)	(used)	weight
c:\kinetics\stat01\36301.prn	95	95	1.0000E+00
c:\kinetics\stat01\36305.prn	85	85	1.0000E+00
c:\kinetics\stat01\36350.prn	109	109	1.0000E+00

Title line of data files:

W=32 N=3 54.2 C/Hr. MaxFid= 5672E-1 Int =20504097E-1 Sample 363

W=21 N=3 4.6 C/Mn. MaxFid= 2185E-0 Int =1667612E-0 Sample 363

W=12 N=3 43.8 C/Mn. MaxFid=11694E-0 Int =938699E-0 Sample 363

Friedman-type analysis at fraction reacted = x

(Valid only if data extend to nearly complete reaction)

x	ln[A(1-x)^n]	A(for n=1) (s^-1)	E (cal/mol)	E std.err. (cal/mol)
.1	3.0634E+01	2.238E+13	51868.	3620.
.2	2.7934E+01	1.693E+12	48176.	2398.
.3	2.8018E+01	2.104E+12	48455.	2114.
.4	2.8350E+01	3.420E+12	49171.	1890.
.5	2.8642E+01	5.497E+12	49909.	1742.
.6	2.8801E+01	8.055E+12	50555.	1718.
.7	2.8847E+01	1.125E+13	51201.	1694.
.8	2.8574E+01	1.283E+13	51668.	1657.
.9	2.8493E+01	2.367E+13	53223.	2564.

Mean approximate A and E over fraction-reacted interval from 0 to x

(Valid only if data extend to nearly complete reaction)

x	A (s^-1)	E (cal/mol)	E std.err. (cal/mol)
.1	5.4272E+15	54814.	1509.
.2	1.6160E+14	51716.	2304.
.3	2.7042E+13	50317.	2477.
.4	1.1131E+13	49973.	2386.
.5	5.4738E+12	49814.	2041.
.6	3.3476E+12	49975.	2041.
.7	2.0257E+12	50219.	1773.
.8	1.2428E+12	50713.	1902.
.9	4.9105E+11	51228.	1801.

Interpolation from parabolic fit of Tmax vs. log(Heating rate):

Tmax = 476.14 C at Heating rate = 25 C/min

Interpolation from linear fit of FWHH vs. log(Heating rate):

FWHH = 53.47 C at Heating rate = 25 C/min

Interpolation from linear fit of Asymmetry vs. log(Heating rate):

Asymmetry = .809 at Heating rate = 25 C/min

Approximate fit of disk data to a single first-order reaction:

Data	Heating rate	Tmax	Exp.FWHH	Cal.FWHH	Exp./Calc.
------	--------------	------	----------	----------	------------

Asymmetry

	(C/min)	(C)	(C)	(C)	
1	8.9826E-01	410.05	46.39	45.69	1.01536
.9731					
2	4.5854E+00	439.31	51.35	49.89	1.02923
.8749					
3	4.8055E+01	491.41	54.26	57.02	.95162
.7845					

A(s⁻¹) = 1.4987E+12
 E(cal/mol) = 4.7764E+04 (std. err. = 1.410E+03)
 S(%E) = 3.6838E-01
 n(order) = 1.0000e+00

Fitting method: Discrete (option 1)
 Least squares of: Relative Rates
 Error tolerance for initial search: 1.0000E-01
 Error tolerance for final convergence: 1.0000E-02
 Thermal history: Constant heating rate (max. rel. std. dev. = 1.155E-03)

Initial minimum frequency factor(s⁻¹): 1.4987E+11
 Initial maximum frequency factor(s⁻¹): 1.4987E+13

Results

Frequency factor = 7.6403E+12 s⁻¹

Percent	Activation energy (cal/mol)
.07	41000.
.11	42000.
.42	43000.
.00	44000.
.00	45000.
.00	46000.
.00	47000.
.00	48000.
.00	49000.
80.40	50000.
.00	51000.
16.42	52000.
.36	53000.
.92	54000.
.00	55000.
1.30	56000.

Least squares exit: successful completion
 Sum of squares of weighted normalized rate residuals: 2.0000E-01
 Sum of squares of weighted integrated rate residuals: 3.1594E-02

Time(s)	Temp(C)	Exp.Rate	Calc.Rate	Exp.Cum.
Calc.Cum.				

Data file: c:\kinetics\stat01\36301.prn
 SFACT = 3.6283E+06, WTR = 3.5883E+03, WTI = 1.0000E+00

2.4000E+03	2.9385E+02	1.8935E-06	2.5561E-06	0.0000E+00
0.0000E+00				
2.5440E+03	2.9615E+02	2.1773E-06	2.7445E-06	2.9310E-04
3.8098E-04				

Sample 364

Code Version: 2.43

Output File: c:\kinetics\stat01\364.out

Data file	Number of data		Group
	(total)	(used)	weight
c:\kinetics\stat01\36401.prn	96	96	1.0000E+00
c:\kinetics\stat01\36405.prn	84	84	1.0000E+00
c:\kinetics\stat01\36450.prn	106	106	1.0000E+00

Title line of data files:

W=35 N=3 -0.9 C/Hr. MaxFid= 2731E-1 Int =10804985E-1 Sample 364

W=21 N=3 4.6 C/Mn. MaxFid= 1019E-0 Int =763842E-0 Sample 364

W=10 N=3 44.0 C/Mn. MaxFid= 4968E-0 Int =396832E-0 Sample 364

Friedman-type analysis at fraction reacted = x

(Valid only if data extend to nearly complete reaction)

x	$\ln[A(1-x)^n]$	A (for n=1) (s ⁻¹)	E (cal/mol)	E std.err. (cal/mol)
.1	3.0420E+01	1.806E+13	51124.	293.
.2	3.0874E+01	3.200E+13	51889.	2257.
.3	3.0694E+01	3.056E+13	51848.	2324.
.4	3.0884E+01	4.312E+13	52397.	2265.
.5	3.1319E+01	7.996E+13	53380.	2288.
.6	3.1898E+01	1.782E+14	54704.	2391.
.7	3.2640E+01	4.991E+14	56464.	2625.
.8	3.4582E+01	5.222E+15	60383.	4478.
.9	3.5086E+01	1.728E+16	62935.	5042.

Mean approximate A and E over fraction-reacted interval from 0 to x

(Valid only if data extend to nearly complete reaction)

x	A (s ⁻¹)	E (cal/mol)	E std.err. (cal/mol)
.1	3.7847E+15	53903.	2003.
.2	4.2048E+14	52597.	143.
.3	1.5079E+14	52279.	1054.
.4	6.1026E+13	51932.	1311.
.5	4.4623E+13	52359.	1640.
.6	3.4431E+13	52883.	1841.
.7	3.1815E+13	53777.	2078.
.8	4.0823E+13	55428.	2585.
.9	8.8646E+13	58590.	4191.

Interpolation from parabolic fit of Tmax vs. log(Heating rate):

Tmax = 468.46 C at Heating rate = 25 C/min

Interpolation from linear fit of FWHH vs. log(Heating rate):

FWHH = 53.89 C at Heating rate = 25 C/min

Interpolation from linear fit of Asymmetry vs. log(Heating rate):

Asymmetry = .859 at Heating rate = 25 C/min

Approximate fit of disk data to a single first-order reaction:

Data Asymmetry	Heating rate (C/min)	Tmax (C)	Exp.FWHH (C)	Cal.FWHH (C)	Exp./Calc.
1 1.0650	8.9744E-01	406.53	47.63	43.18	1.10301
2 .9886	4.6386E+00	433.54	50.68	46.98	1.07881
3 .8078	4.8148E+01	483.03	55.14	53.29	1.03465

$A(s^{-1}) = 1.1248E+13$
 $E(\text{cal/mol}) = 5.0197E+04$ (std. err. = $2.134E+03$)
 $S(\%E) = 1.0456E+00$
 $n(\text{order}) = 1.0000E+00$

Fitting method: Discrete (option 1)
Least squares of: Relative Rates
Error tolerance for initial search: $1.0000E-01$
Error tolerance for final convergence: $1.0000E-02$
Thermal history: Constant heating rate (max. rel. std. dev. = $1.156E-03$)

Initial minimum frequency factor(s^{-1}): $1.1248E+12$
Initial maximum frequency factor(s^{-1}): $1.1248E+14$

Results

Frequency factor = $5.0215E+13 s^{-1}$
Percent Activation energy (cal/mol)

.05	43000.
.19	44000.
.09	45000.
.44	46000.
.00	47000.
.00	48000.
.00	49000.
.00	50000.
.00	51000.
65.70	52000.
3.19	53000.
24.16	54000.
.00	55000.
4.80	56000.
.00	57000.
.00	58000.
.00	59000.
1.39	60000.

Least squares exit: successful completion

Sum of squares of weighted normalized rate residuals: $1.5290E-01$
Sum of squares of weighted integrated rate residuals: $2.6156E-02$

Time(s)	Temp(C)	Exp.Rate	Calc.Rate	Exp.Cum.
Calc.Cum.				

Data file: c:\kinetics\stat01\36401.prn
SFACT = $3.9797E+06$, WTR = $3.9280E+03$, WTI = $1.0000E+00$

$2.7840E+03$ $2.9925E+02$ $2.2942E-06$ $3.7379E-06$ $0.0000E+00$

Sample 365

Code Version: 2.43

Output File: c:\kinetics\stat01\365.out

Data file	Number of data (total)	(used)	Group weight
c:\kinetics\stat01\36501.prn	113	113	1.0000E+00
c:\kinetics\stat01\36505.prn	116	116	1.0000E+00
c:\kinetics\stat01\36550.prn	106	106	1.0000E+00

Title line of data files:

W=33 N=3 -1.2 C/Hr. MaxFid= 4479E-1 Int =21445093E-1 Sample 365

W=20 N=3 4.5 C/Mn. MaxFid= 1433E-0 Int =1440358E-0 Sample 365

W=9 N=3 43.6 C/Mn. MaxFid= 6647E-0 Int =649304E-0 Sample 365

Friedman-type analysis at fraction reacted = x

(Valid only if data extend to nearly complete reaction)

x	ln[A(1-x)^n]	A(for n=1) (s^-1)	E (cal/mol)	E std.err. (cal/mol)
.1	2.8138E+01	1.845E+12	47493.	174.
.2	2.9400E+01	7.330E+12	49624.	282.
.3	2.9575E+01	9.986E+12	50263.	63.
.4	2.9637E+01	1.239E+13	50749.	9.
.5	2.9872E+01	1.880E+13	51543.	127.
.6	3.0066E+01	2.855E+13	52387.	476.
.7	3.0205E+01	4.374E+13	53332.	1017.
.8	3.0415E+01	8.093E+13	54741.	1953.
.9	3.1026E+01	2.982E+14	57699.	4951.

Mean approximate A and E over fraction-reacted interval from 0 to x

(Valid only if data extend to nearly complete reaction)

x	A (s^-1)	E (cal/mol)	E std.err. (cal/mol)
.1	2.2181E+13	46435.	1020.
.2	1.8960E+13	47909.	521.
.3	1.5329E+13	48812.	405.
.4	1.0823E+13	49336.	500.
.5	8.5260E+12	49958.	238.
.6	7.6079E+12	50782.	73.
.7	5.2145E+12	51334.	331.
.8	4.2121E+12	52404.	817.
.9	3.9850E+12	54508.	2092.

Interpolation from parabolic fit of Tmax vs. log(Heating rate):

Tmax = 468.65 C at Heating rate = 25 C/min

Interpolation from linear fit of FWHH vs. log(Heating rate):

FWHH = 68.40 C at Heating rate = 25 C/min

Interpolation from linear fit of Asymmetry vs. log(Heating rate):

Asymmetry = .877 at Heating rate = 25 C/min

Approximate fit of disk data to a single first-order reaction:

Data	Heating rate	Tmax	Exp.FWHH	Cal.FWHH	Exp./Calc.
------	--------------	------	----------	----------	------------

Asymmetry

	(C/min)	(C)	(C)	(C)	
1	8.9995E-01	405.33	61.86	43.60	1.41887
.8543					
2	4.5361E+00	434.52	65.69	47.41	1.38560
.8761					
3	4.8022E+01	482.76	69.43	53.92	1.28772
.8773					

A(s⁻¹) = 7.1068E+12
 E(cal/mol) = 4.9775E+04 (std. err. = 2.762E+02)
 S(%E) = 2.6452E+00
 n(order) = 1.0000e+00

Fitting method: Discrete (option 1)
 Least squares of: Relative Rates
 Error tolerance for initial search: 1.0000E-01
 Error tolerance for final convergence: 1.0000E-02
 Thermal history: Constant heating rate (max. rel. std. dev. = 1.041E-03)

Initial minimum frequency factor(s⁻¹): 7.1068E+11
 Initial maximum frequency factor(s⁻¹): 7.1068E+13

Results

Frequency factor = 9.7710E+12 s⁻¹
 Percent Activation energy (cal/mol)

.05	41000.
.17	42000.
.00	43000.
.33	44000.
.19	45000.
2.04	46000.
2.82	47000.
4.04	48000.
17.87	49000.
32.24	50000.
19.25	51000.
11.78	52000.
1.83	53000.
4.70	54000.
.00	55000.
.75	56000.
.70	57000.
.00	58000.
1.26	59000.

Least squares exit: successful completion
 Sum of squares of weighted normalized rate residuals: 5.8294E-02
 Sum of squares of weighted integrated rate residuals: 7.4633E-03

Time(s)	Temp(C)	Exp.Rate	Calc.Rate	Exp.Cum.
Calc.Cum.				

Data file: c:\kinetics\stat01\36501.prn
 SFACT = 4.8051E+06, WTR = 4.7936E+03, WTI = 1.0000E+00

2.1120E+03 2.9026E+02 1.5567E-06 2.6773E-06 0.0000E+00

Sample 366

Code Version: 2.43

Output File: c:\kinetics\stat01\366.out

Data file	Number of data		Group
	(total)	(used)	weight
c:\kinetics\stat01\36601.prn	89	89	1.0000E+00
c:\kinetics\stat01\36605.prn	87	87	1.0000E+00
c:\kinetics\stat01\36650.prn	94	94	1.0000E+00

Title line of data files:

W=48 N=3 -1.3 C/Hr. MaxFid= 6197E-1 Int =23149937E-1 Sample 366

W=22 N=3 4.5 C/Mn. MaxFid= 1122E-0 Int =888015E-0 Sample 366

W=11 N=3 46.8 C/Mn. MaxFid= 6262E-0 Int =488961E-0 Sample 366

Friedman-type analysis at fraction reacted = x

(Valid only if data extend to nearly complete reaction)

x	ln[A(1-x)^n]	A(for n=1) (s^-1)	E (cal/mol)	E std.err. (cal/mol)
.1	2.9887E+01	1.060E+13	50534.	1644.
.2	2.9662E+01	9.525E+12	50384.	420.
.3	2.9480E+01	9.075E+12	50343.	95.
.4	2.9666E+01	1.276E+13	50887.	239.
.5	2.9846E+01	1.832E+13	51492.	227.
.6	2.9983E+01	2.626E+13	52147.	158.
.7	3.0022E+01	3.642E+13	52815.	78.
.8	2.9785E+01	4.308E+13	53372.	603.
.9	2.9373E+01	5.707E+13	54430.	1347.

Mean approximate A and E over fraction-reacted interval from 0 to x

(Valid only if data extend to nearly complete reaction)

x	A (s^-1)	E (cal/mol)	E std.err. (cal/mol)
.1	4.7546E+15	54394.	418.
.2	2.7781E+14	52200.	797.
.3	7.0155E+13	51408.	653.
.4	2.8803E+13	51088.	635.
.5	1.6061E+13	51137.	409.
.6	9.7831E+12	51331.	232.
.7	5.9470E+12	51604.	143.
.8	3.2970E+12	51981.	114.
.9	1.7862E+12	52996.	262.

Interpolation from parabolic fit of Tmax vs. log(Heating rate):

Tmax = 472.72 C at Heating rate = 25 C/min

Interpolation from linear fit of FWHH vs. log(Heating rate):

FWHH = 55.75 C at Heating rate = 25 C/min

Interpolation from linear fit of Asymmetry vs. log(Heating rate):

Asymmetry = .798 at Heating rate = 25 C/min

Approximate fit of disk data to a single first-order reaction:

Data	Heating rate	Tmax	Exp.FWHH	Cal.FWHH	Exp./Calc.
------	--------------	------	----------	----------	------------

Asymmetry

	(C/min)	(C)	(C)	(C)	
1	9.0235E-01	408.61	48.97	44.09	1.11081
.9205					
2	4.5453E+00	438.46	53.03	47.96	1.10552
.8492					
3	5.0307E+01	487.93	56.87	54.73	1.03914
.7767					

A(s⁻¹) = 5.9090E+12
 E(cal/mol) = 4.9587E+04 (std. err. = 2.293E+01)
 S(%E) = 1.1563E+00
 n(order) = 1.0000e+00

Fitting method: Discrete (option 1)
 Least squares of: Relative Rates
 Error tolerance for initial search: 1.0000E-01
 Error tolerance for final convergence: 1.0000E-02
 Thermal history: Constant heating rate (max. rel. std. dev. = 1.074E-03)

Initial minimum frequency factor(s⁻¹): 5.9090E+11
 Initial maximum frequency factor(s⁻¹): 5.9090E+13

Results

Frequency factor = 1.0688E+13 s⁻¹
 Percent Activation energy (cal/mol)

.02	42000.
.24	43000.
.00	44000.
.00	45000.
.00	46000.
.00	47000.
.00	48000.
.00	49000.
55.75	50000.
24.82	51000.
13.55	52000.
1.68	53000.
3.32	54000.
.00	55000.
.00	56000.
.62	57000.

Least squares exit: successful completion

Sum of squares of weighted normalized rate residuals: 3.8772E-02
 Sum of squares of weighted integrated rate residuals: 1.3684E-02

Time(s)	Temp(C)	Exp.Rate	Calc.Rate	Exp.Cum.
Calc.Cum.				

Data file: c:\kinetics\stat01\36601.prn
 SFACT = 3.7433E+06, WTR = 3.7210E+03, WTI = 1.0000E+00

3.4560E+03	3.0928E+02	1.9314E-06	3.6298E-06	0.0000E+00
0.0000E+00				
3.6000E+03	3.1149E+02	2.0623E-06	3.8317E-06	2.8755E-04
5.3625E-04				

Sample 367

Code Version: 2.43

Output File: c:\kinetics\stat01\367.out

Data file	Number of data		Group
	(total)	(used)	weight
c:\kinetics\stat01\36701.prn	79	79	1.0000E+00
c:\kinetics\stat01\36705.prn	72	72	1.0000E+00
c:\kinetics\stat01\36750b.prn	100	100	1.0000E+00

Title line of data files:

W=33 N=3 27.5 C/Hr. MaxFid= 4257E-1 Int =14448126E-1 Sample 367

W=11 N=3 4.6 C/Mn. MaxFid= 1734E-0 Int =1271381E-0 Sample 367

W=9 N=3 43.3 C/Mn. MaxFid= 5262E-0 Int =408747E-0 Sample 367

Friedman-type analysis at fraction reacted = x

(Valid only if data extend to nearly complete reaction)

x	ln[A(1-x)^n]	A(for n=1) (s^-1)	E (cal/mol)	E std.err. (cal/mol)
.1	3.0643E+01	2.259E+13	51588.	3336.
.2	2.9311E+01	6.705E+12	49738.	2358.
.3	2.9261E+01	7.291E+12	49840.	2160.
.4	2.9530E+01	1.114E+13	50471.	2197.
.5	2.9807E+01	1.762E+13	51181.	2125.
.6	3.0115E+01	2.996E+13	52031.	2100.
.7	3.0316E+01	4.886E+13	52871.	2202.
.8	3.0456E+01	8.429E+13	53883.	2422.
.9	3.1476E+01	4.675E+14	56905.	4309.

Mean approximate A and E over fraction-reacted interval from 0 to x

(Valid only if data extend to nearly complete reaction)

x	A (s^-1)	E (cal/mol)	E std.err. (cal/mol)
.1	5.3656E+16	57733.	3158.
.2	8.4398E+14	53712.	2884.
.3	1.3116E+14	52201.	2747.
.4	4.7742E+13	51683.	2742.
.5	2.2756E+13	51475.	2638.
.6	1.2377E+13	51464.	2564.
.7	8.4686E+12	51882.	2327.
.8	4.4271E+12	52118.	2277.
.9	3.4695E+12	53566.	2903.

Interpolation from parabolic fit of Tmax vs. log(Heating rate):

Tmax = 470.97 C at Heating rate = 25 C/min

Interpolation from linear fit of FWHH vs. log(Heating rate):

FWHH = 52.71 C at Heating rate = 25 C/min

Interpolation from linear fit of Asymmetry vs. log(Heating rate):

Asymmetry = .753 at Heating rate = 25 C/min

Approximate fit of disk data to a single first-order reaction:

Data	Heating rate	Tmax	Exp.FWHH	Cal.FWHH	Exp./Calc.
------	--------------	------	----------	----------	------------

Asymmetry

	(C/min)	(C)	(C)	(C)	
1	8.9706E-01	407.04	43.38	44.38	.97746
1.0573					
2	4.5485E+00	434.82	50.05	48.34	1.03533
.8500					
3	4.7057E+01	485.40	53.64	55.02	.97482
.7190					

A(s⁻¹) = 3.7778E+12
 E(cal/mol) = 4.8743E+04 (std. err. = 1.810E+03)
 S(%E) = 2.4484E-01
 n(order) = 1.0000e+00

Fitting method: Discrete (option 1)
 Least squares of: Relative Rates
 Error tolerance for initial search: 1.0000E-01
 Error tolerance for final convergence: 1.0000E-02
 Thermal history: Constant heating rate (max. rel. std. dev. = 1.443E-03)

Initial minimum frequency factor(s⁻¹): 3.7778E+11
 Initial maximum frequency factor(s⁻¹): 3.7778E+13

Results

Frequency factor = 1.9678E+13 s⁻¹

Percent	Activation energy (cal/mol)
.11	43000.
.00	44000.
.00	45000.
.00	46000.
.00	47000.
.00	48000.
.00	49000.
.00	50000.
80.28	51000.
3.74	52000.
14.89	53000.
.00	54000.
.00	55000.
.00	56000.
.97	57000.

Least squares exit: successful completion
 Sum of squares of weighted normalized rate residuals: 2.5631E-01
 Sum of squares of weighted integrated rate residuals: 5.5659E-02

Time(s)	Temp(C)	Exp.Rate	Calc.Rate	Exp.Cum.
Calc.Cum.				

Data file: c:\kinetics\stat01\36701.prn
 SFACT = 3.4085E+06, WTR = 3.3725E+03, WTI = 1.0000E+00

3.7440E+03	3.1311E+02	2.7959E-06	3.5986E-06	0.0000E+00
0.0000E+00				
3.8880E+03	3.1519E+02	3.0365E-06	3.5905E-06	4.1994E-04
5.1644E-04				
4.0320E+03	3.1716E+02	3.2272E-06	3.5806E-06	8.7092E-04

Sample 368

Code Version: 2.43

Output File: c:\kinetics\stat01\368.out

Data file	Number of data (total)	Number of data (used)	Group weight
c:\kinetics\stat01\36801.prn	93	93	1.0000E+00
c:\kinetics\stat01\36805.prn	90	90	1.0000E+00
c:\kinetics\stat01\36850.prn	106	106	1.0000E+00

Title line of data files:

W=20 N=3 -1.1 C/Hr. MaxFid= 6328E-1 Int =23125652E-1 Sample 368

W=20 N=3 4.6 C/Mn. MaxFid= 2360E-0 Int =1827621E-0 Sample 368

W=12 N=3 43.6 C/Mn. MaxFid=15226E-0 Int =1204935E-0 Sample 368

Friedman-type analysis at fraction reacted = x

(Valid only if data extend to nearly complete reaction)

x	ln[A(1-x)^n]	A (for n=1) (s^-1)	E (cal/mol)	E std.err. (cal/mol)
.1	2.9661E+01	8.464E+12	50496.	3357.
.2	2.9199E+01	5.997E+12	49914.	2144.
.3	2.9526E+01	9.501E+12	50542.	1734.
.4	2.9781E+01	1.430E+13	51174.	1601.
.5	2.9958E+01	2.049E+13	51776.	1437.
.6	3.0086E+01	2.911E+13	52408.	1365.
.7	3.0167E+01	4.211E+13	53128.	1365.
.8	3.0143E+01	6.164E+13	53998.	1260.
.9	2.9963E+01	1.030E+14	55437.	1519.

Mean approximate A and E over fraction-reacted interval from 0 to x

(Valid only if data extend to nearly complete reaction)

x	A (s^-1)	E (cal/mol)	E std.err. (cal/mol)
.1	6.3702E+14	52019.	595.
.2	9.3537E+13	50978.	1879.
.3	3.4648E+13	50642.	2142.
.4	2.0536E+13	50800.	2069.
.5	1.3612E+13	51068.	1925.
.6	8.8519E+12	51333.	1625.
.7	5.7777E+12	51691.	1744.
.8	3.6516E+12	52248.	1527.
.9	2.0043E+12	53289.	1144.

Interpolation from parabolic fit of Tmax vs. log(Heating rate):

Tmax = 474.49 C at Heating rate = 25 C/min

Interpolation from linear fit of FWHH vs. log(Heating rate):

FWHH = 53.65 C at Heating rate = 25 C/min

Interpolation from linear fit of Asymmetry vs. log(Heating rate):

Asymmetry = .874 at Heating rate = 25 C/min

Approximate fit of disk data to a single first-order reaction:

Data	Heating rate	Tmax	Exp.FWHH	Cal.FWHH	Exp./Calc.
Asymmetry	(C/min)	(C)	(C)	(C)	
1	9.0213E-01	411.18	47.09	43.99	1.07031
.9084					
2	4.5869E+00	439.11	52.57	47.86	1.09821
.9428					
3	4.7865E+01	489.03	54.01	54.40	.99295
.8471					

A(s⁻¹) = 7.0318E+12
 E(cal/mol) = 4.9913E+04 (std. err. = 1.580E+03)
 S(%E) = 7.6068E-01
 n(order) = 1.0000e+00

Fitting method: Discrete (option 1)
 Least squares of: Relative Rates
 Error tolerance for initial search: 1.0000E-01
 Error tolerance for final convergence: 1.0000E-02
 Thermal history: Constant heating rate (max. rel. std. dev. = 1.722E-03)

Initial minimum frequency factor(s⁻¹): 7.0318E+11
 Initial maximum frequency factor(s⁻¹): 7.0318E+13

Results

Frequency factor = 1.7543E+13 s⁻¹
 Percent Activation energy (cal/mol)

.00	42000.
.10	43000.
.32	44000.
.00	45000.
.00	46000.
.00	47000.
.00	48000.
.00	49000.
.00	50000.
68.45	51000.
12.14	52000.
15.06	53000.
.00	54000.
3.30	55000.
.00	56000.
.00	57000.
.62	58000.

Least squares exit: successful completion
 Sum of squares of weighted normalized rate residuals: 1.2281E-01
 Sum of squares of weighted integrated rate residuals: 1.7951E-02

Time(s)	Temp(C)	Exp.Rate	Calc.Rate	Exp.Cum.
Calc.Cum.				

Data file: c:\kinetics\stat01\36801.prn
 SFACT = 3.6576E+06, WTR = 3.6477E+03, WTI = 1.0000E+00

3.7920E+03	3.1440E+02	3.3164E-06	5.5617E-06	0.0000E+00
0.0000E+00				

Sample 369

Code Version: 2.43

Output File: c:\kinetics\stat01\369.out

Data file	Number of data (total)	Group (used)	weight
c:\kinetics\stat01\36901.prn	100	100	1.0000E+00
c:\kinetics\stat01\36905.prn	80	80	1.0000E+00
c:\kinetics\stat01\36950.prn	129	129	1.0000E+00

Title line of data files:

W=25 N=3 53.9 C/Hr. MaxFid= 1935E-1 Int =8018848E-1 Sample 369

W=20 N=3 4.6 C/Mn. MaxFid= 998E-0 Int =769702E-0 Sample 369

W=13 N=3 44.0 C/Mn. MaxFid= 8040E-0 Int =621986E-0 Sample 369

Friedman-type analysis at fraction reacted = x

(Valid only if data extend to nearly complete reaction)

x	ln[A(1-x)^n]	A(for n=1) (s^-1)	E (cal/mol)	E std.err. (cal/mol)
.1	2.9881E+01	1.055E+13	50320.	941.
.2	3.0701E+01	2.693E+13	51639.	2272.
.3	3.0895E+01	3.738E+13	52138.	2719.
.4	3.0943E+01	4.572E+13	52472.	2428.
.5	3.1582E+01	1.039E+14	53753.	2233.
.6	3.2568E+01	3.483E+14	55678.	2681.
.7	3.4416E+01	2.947E+15	59105.	4188.
.8	3.4949E+01	7.533E+15	60941.	4747.
.9	3.4672E+01	1.143E+16	62386.	5256.

Mean approximate A and E over fraction-reacted interval from 0 to x

(Valid only if data extend to nearly complete reaction)

x	A (s^-1)	E (cal/mol)	E std.err. (cal/mol)
.1	5.4818E+15	54144.	2749.
.2	4.5409E+14	52564.	25.
.3	1.3640E+14	52067.	1393.
.4	5.9496E+13	51866.	1615.
.5	3.6810E+13	52070.	1588.
.6	3.5832E+13	52930.	1857.
.7	4.7044E+13	54336.	2387.
.8	7.8318E+13	56371.	3306.
.9	1.3415E+14	59217.	4539.

Interpolation from parabolic fit of Tmax vs. log(Heating rate):

Tmax = 468.49 C at Heating rate = 25 C/min

Interpolation from linear fit of FWHH vs. log(Heating rate):

FWHH = 52.40 C at Heating rate = 25 C/min

Interpolation from linear fit of Asymmetry vs. log(Heating rate):

Asymmetry = .833 at Heating rate = 25 C/min

Approximate fit of disk data to a single first-order reaction:

Data	Heating rate	Tmax	Exp.FWHH	Cal.FWHH	Exp./Calc.
Asymmetry	(C/min)	(C)	(C)	(C)	
1	9.0023E-01	405.44	51.64	43.77	1.17982
1.0656					
2	4.6058E+00	433.46	50.62	47.65	1.06221
.9349					
3	4.9249E+01	483.60	53.12	54.26	.97908
.7917					

$A(s^{-1}) = 6.2547E+12$
 $E(cal/mol) = 4.9346E+04$ (std. err. = $1.468E+03$)
 $S(\%E) = 9.0234E-01$
 $n(order) = 1.0000e+00$

Fitting method: Discrete (option 1)
Least squares of: Relative Rates
Error tolerance for initial search: $1.0000E-01$
Error tolerance for final convergence: $1.0000E-02$
Thermal history: Constant heating rate (max. rel. std. dev. = $1.563E-03$)

Initial minimum frequency factor(s^{-1}): $6.2547E+11$
Initial maximum frequency factor(s^{-1}): $6.2547E+13$

Results

Frequency factor = $5.5349E+13 s^{-1}$
Percent Activation energy (cal/mol)

.00	43000.
.08	44000.
.43	45000.
.00	46000.
.77	47000.
.26	48000.
.00	49000.
.00	50000.
.00	51000.
58.33	52000.
6.33	53000.
26.37	54000.
.00	55000.
5.23	56000.
.75	57000.
.15	58000.
.00	59000.
.00	60000.
1.29	61000.

Least squares exit: successful completion
Sum of squares of weighted normalized rate residuals: $2.3657E-01$
Sum of squares of weighted integrated rate residuals: $4.3515E-02$

Time(s)	Temp(C)	Exp.Rate	Calc.Rate	Exp.Cum.
Calc.Cum.				

Data file: c:\kinetics\stat01\36901.prn
SFACT = $4.1705E+06$, WTR = $4.0390E+03$, WTI = $1.0000E+00$