

VI. U Z U P E Ł N I E N I E

**dotyczące programów obliczeń
związanych z rozprawą doktorską pt.:
"Kinetyka rekombinacji atomowego
wodoru na filmach metali przejściowych"**

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F-B.133/75/2



70000000012835



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Uzupełnienie to zostało opracowane ze względu na stosowanie metody Smitha - Linnetta w Zakładzie Katalizy na Metalach IChF PAN. Przeznaczone jest ono dla przyszłych użytkowników tej metody. Załączono programy służące do analizy danych doświadczalnych związanych z kinetyką rekombinacji atomowego wodoru. Podano również sposób przygotowania danych do obliczeń oraz sposób uruchamiania programów. Napisane są one w języku Algol 1204; umożliwiają dokonywanie obliczeń na maszynie cyfrowej Odra 1204.

VI. 1. Program analizy danych doświadczalnych metodą Smitha - Linnetta

A. Algorytm.

Jest on szczegółowo opisany w punkcie 8.4.1. rozprawy.

B. Postać danych.

Należy je wprowadzać w następującej kolejności:

k - numer eksperymentu;

n - liczba pomiarów aktywności badanej powierzchni;

ϵ - parametr ϵ/k potencjału Lennarda - Jonesa (6-12) dla oddziaływania $H - H_2$ [°K];

σ - parametr σ potencjału Lennarda - Jonesa (6-12) dla oddziaływania $H - H_2$ [Å];

R - promień wewnętrzny cylindrycznej wkładki [cm];

m_i - tabela liczb punktów doświadczalnych w kolejnych pomiarach ($i = 1, 2, \dots, n$);

p_i - tabela ciśnień wodoru w czasie kolejnych pomiarów ($i = 1, 2, \dots, n$) [10^{-3} Tr];

$temp_i$ - tabela kolejnych temperatur ($i = 1, 2, \dots, n$) [°C];

X_{ij} - tabela położzeń ruchomej sondy katalitycznej dla kolej-

nych pomiarów. (odległości spoiny pokrytej srebrem od dowolnie ustalonego punktu w bocznym ramieniu ;

$i = 1, 2, \dots, n ; j = 1, 2, \dots, m_1$) [cm] ;

E_{ij} - siły termoelektryczne termopary miedź - konstantan odpowiadające położeniom X_{ij} ($i = 1, 2, \dots, n ; j = 1, 2, \dots, m_1$) [10^{-5} v] ,

C. Uruchamianie programu.

Po starcie na monitorze pojawi się napis "wait dane". Należy wówczas wczytać zestaw danych po naciśnięciu dowolnego klawisza na monitorze. Sygnałem końca obliczeń jest powtórne pojawienie się napisu "wait dane".

begin

integer k, n, i, j, v;

real eps, sigma, R, p1, p2, a, b, c, d, alfa, T, Tr, const, omega, h, Eo, Et, xb, ga, gb;

ZZ:wait('dane');

read(k, n, eps, sigma, R);

begin

integer array m[1:n];

array p, temp[1:n]; read(m, p, temp); v=0;

for i=1 step 1 until n do v=v+m[i];

begin

array X, E, delta[1:v], WW[1:4];

real procedure F(x);

value x;

real x;

begin

real p;

integer i;

p=0;

for i=1 step 1 until 4 do p=p*x+WW[i];

F=p*x

end F;

WW[1]:= 1.48098339₁₀⁻¹¹;

WW[2]:= -3.60121584₁₀⁻⁸;

WW[3]:= 4.62395134₁₀⁻⁵;

WW[4]:= 3.85014117₁₀⁻²;

```

read(X,E); h:=0.5; v:=0;
for i:=1 step 1 until n do
  begin
    Eo:=F(temp[i]);
    for j:=1 step 1 until m[i] do
      begin
        xb:=0;
        Et:=Eo+E[v+j]/100;
        if Et=0 then go to ZD;
        if Et<0 then h:=-abs(h) else h:=abs(h);
        if F(xb) -Et<0 then go to ZB;
        ZA:if F(xb) -Et>0 then
          begin
            xb:=xb+h; go to ZA
          end;
          ga:=xb; gb:=xb-h; go to ZC;
        ZB:if F(xb) -Et<0 then
          begin
            xb:=xb+h; go to ZB
          end;
          gb:=xb; ga:=xb-h;
        ZC:xb:=(ga+gb)/2;
        if F(xb) -Et>0 then gb:=xb else ga:=xb;
        if abs(ga-gb)>10-8 then go to ZC;
        ZD:delta[v+j]:=xb-temp[i]
      end
    end
  end

```

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        end;
        v:=v+m[i]
    end;
    line(1);
    print('Experiment no'); format('11'); print(k);
    line(2);
print('No. of points: T, p, gamma, 1000/T, ln(gamma)
[deg-K], [torr], Smith-Linnett
analysis');
format(' ?11 11.1 11.1 1.11 1.1110-1 1.11 1.1110-1 ');
    line(1); v:=0;
    for i:=1 step 1 until n do
        begin
            T:=temp[i] + 273; Tr:=T/eps;
            omega:=1.075*exp(-0.1615*ln(Tr))+2*exp(-0.3213779166*ln(10*Tr)*ln(10*Tr));
            a:=b:=c:=d:=0;
            for j:=1 step 1 until m[i] do
                begin
                    a:=a+X[v+j];
                    b:=b+ln(delta[v+j]);
                    c:=c+X[v+j]*X[v+j];
                    d:=d+X[v+j]*ln(delta[v+j])
                end;
            p1:=m[i]*d-a*b; p2:=m[i]*c-a*a; alfa=p1/p2;
            const:=0.2378043918*R/(p[i]*sigma*sigma*omega);

```



```
Tr:=const×T×alfa×alfa; print(i,T,p[i]/1000,Tr,1000/T,ln(Tr));  
v:=v+m[i]  
    end;  
line(15);  
go to ZZ  
    end  
    end  
end?
```

VI. 2. Program analizy danych doświadczalnych w oparciu o równanie (6.6)

A. Algorytm.

Jest on szczegółowo opisany w punkcie 8.4.2 rozprawy.

B. Postać danych.

Należy je wprowadzać w następującej kolejności:

k - numer eksperymentu;

n - liczba pomiarów aktywności badanej powierzchni;

eps - parametr ϵ/k potencjału Lennarda - Jonesa (6-12) dla oddziaływania H - H₂ [°K];

sigma - parametr δ potencjału Lennarda - Jonesa dla oddziaływania H - H₂ [$\overset{\circ}{\text{A}}$];

R - wewnętrzny promień cylindrycznej wkładki [cm];

m₁ - tabela liczb punktów doświadczalnych w kolejnych pomiarach (i = 1, 2, ..., n);

p_i - tabela ciśnień wodoru w czasie kolejnych pomiarów (i = 1, 2, ..., n): [10^{-3} Tr];

temp₁ - tabela kolejnych temperatur (i = 1, 2, ..., n) [°C];

X_{1j} - tabela położzeń ruchomej sondy katalitycznej dla kolejnych pomiarów (i = 1, 2, ..., n; j = 1, 2, ..., m₁) [cm].

Pomiarów siły termoelektrycznej dokonywano w następującej kolejności. Początkowo ustawiano spoinę termopary pokrytą srebrem na wysokości przedniej krawędzi cylindrycznej wkładki (w kierunku wyładowań). Położeniu temu odpowiadała największa wartość odległości X. Po zmierzeniu siły termoelektrycznej termoparę cofano maksymalnie do tyłu (najmniejsza wartość X). Następnie dokonywano kilku pomiarów siły termoelektrycznej prze-

suwając termoparę stopniowo do przodu, aż do położenia początkowego. W takiej kolejności należy podawać wartości X_{1j} dla danego i , tj.

$$X_{11} > X_{12} < X_{13} < \dots < X_{1m_1} = X_{11} .$$

E_{1j} - siły termoelektryczne termopary miedź - konstantan odpowiadające położeniom X_{1j} ($i = 1, 2, \dots, n$; $j = 1, 2, \dots, m_1$) [10^{-5} V] .

Na stronie A9 podano przykładowe zestawienie danych do obliczeń. Dane te zebrano podczas eksperymentu nr 34 (film Ni na pyreksie).

C. Uruchamianie programu.

Po starcie należy wczytać tabele wartości $\alpha_i(\delta)$ oraz $\beta_i(\delta)$ zestawione na stronach A10-A21 dla $i = 1, 2, \dots, 30$. Należy je wczytywać kolejno kolumnami. Wielkość $\alpha_i(\delta)$ oznacza i - ty pierwiastek równania $x\delta J_1(x) = J_0(x)$, gdzie $J_k(x)$ jest funkcją Bessela pierwszego rodzaju, k - tego rzędu; δ jest dyfuzyjną liczbą Reynoldsa. Wielkość $\beta_i(\delta)$ dana jest wzorem

$$\beta_i(\delta) = \frac{2}{\alpha_i(1 + \alpha_i^2 \delta^2) J_1(\alpha_i)} .$$

Na monitorze pojawi się napis "wait dane". Należy wówczas wczytać zestaw danych po naciśnięciu dowolnego klawisza na monitorze. Sygnałem końca obliczeń jest pojawienie się na monitorze napisu "END".

D. Przykład przygotowania danych do obliczeń .
Eksperyment 34; Ni/pyreks

k	34											
n	12											
eps	85											
sigma	2.32											
R	1.6											
m_i	6	6	6	6	6	6	6	6	6	6	6	6
p_i	90	90	90	90	90	90	90	90	90	90	90	90
T_i	180	180	90	90	25	25	-28	-28	-58	-58	180	180
x_{ij}	10	3	5	7	9	10	10	10	10	10	10	10
	10	3	5	7	9	10	10	10	10	10	10	10
	10	3	5	7	9	10	10	10	10	10	10	10
	10	3	5	7	9	10	10	10	10	10	10	10
	10	3	5	7	9	10	10	10	10	10	10	10
	10	3	5	7	9	10	10	10	10	10	10	10
	10	3	5	7	9	10	10	10	10	10	10	10
	10	3	5	7	9	10	10	10	10	10	10	10
	10	3	5	7	9	10	10	10	10	10	10	10
	10	3	5	7	9	10	10	10	10	10	10	10
E_{ij}	91.7	12.8	19.9	35.8	66.9	89.5	84.9	14.3	21.5	36.5	64.6	84.2
	84.2	13.1	21.8	37.9	65.3	82.3	79.8	14.5	23.5	39.0	64.3	79.1
	89.2	19.7	31.6	50.3	78.0	93.9	95.5	25.2	37.7	56.2	82.1	97.0
	324.6	271.9	289.7	305.3	319.4	325.8	328.7	275.6	292.6	308.8	323.5	331.6
	316.4	270.4	287.9	302.6	315.6	322.3	326.8	277.2	292.8	308.5	327.0	337.1
	76.1	16.8	23.1	36.9	60.6	75.4	73.4	16.2	22.6	35.8	58.5	68.9

delta	alfa i				
	.125	.250	.500	1	2
1	2.1286385	1.9080788	1.5994492	1.2557837	.9407706
2	4.9383790	4.6018456	4.2909585	4.0794777	3.9593712
3	7.8463581	7.5200705	7.2883889	7.1557992	7.0863809
4	10.8270595	10.5422877	10.3658311	10.2709853	10.2224584
5	13.8566370	13.6124763	13.4718820	13.3983975	13.3611489
6	16.9178805	16.7072688	16.5910330	16.5311589	16.5009499
7	19.9998800	19.8160365	19.7172066	19.6667278	19.6413261
8	23.0958848	22.9334138	22.8475656	22.8039505	22.7820386
9	26.2016519	26.0564403	25.9806148	25.9422289	25.9229648
10	29.3144372	29.1833616	29.1154936	29.0812218	29.0640354
11	32.4324099	32.3130767	32.2516725	32.2207209	32.2052079
12	35.5543114	35.4448615	35.3888077	35.3605915	35.3464552
13	38.6792528	38.5782208	38.5266668	38.5007428	38.4877589
14	41.8065904	41.7128053	41.6650869	41.6411113	41.6291063
15	44.9358479	44.8483613	44.8039506	44.7816515	44.7704881
16	48.0666661	47.9847006	47.9431710	47.9223296	47.9118976
17	51.1987691	51.1216805	51.0826825	51.0631201	51.0533296
18	54.3319421	54.2591907	54.2224347	54.2040036	54.1947802
19	57.4660150	57.3971451	57.3623881	57.3449647	57.3362465
20	60.6008520	60.5354749	60.5025114	60.4859914	60.4777258
21	63.7363428	63.6741251	63.6427796	63.6270740	63.6192164
22	66.8723975	66.8130507	66.7831723	66.7682046	66.7607165
23	70.0089417	69.9522149	69.9236726	69.9093766	69.9022250
24	73.1459137	73.0915871	73.0642668	73.0505849	73.0437407
25	76.2832614	76.2311416	76.2049432	76.1918248	76.1852628
26	79.4209411	79.3708570	79.3456921	79.3330927	79.3267905
27	82.5589153	82.5107148	82.4865052	82.4743853	82.4683231
28	85.6971522	85.6506996	85.6273755	85.6156999	85.6098601
29	88.8356242	88.7907979	88.7682968	88.7570342	88.7514011
30	91.9743076	91.9309981	91.9092641	91.8983861	91.8929455

		alfa i				
delta		4	8	16	32	64
i						
1		.6855876	.4922895	.3508093	.2490266	.1764320
2		3.8963163	3.8641795	3.8479813	3.8398528	3.8357816
3		7.0511167	7.0333797	7.0244895	7.0200396	7.0178135
4		10.1980073	10.1857470	10.1796096	10.1765394	10.1750039
5		13.3424401	13.3330701	13.3283819	13.3260372	13.3248646
6		16.4858004	16.4782174	16.4744242	16.4725272	16.4715787
7		19.6285985	19.6222298	19.6190444	19.6174516	19.6166551
8		22.7710655	22.7655758	22.7628303	22.7614574	22.7607709
9		25.9133212	25.9084972	25.9060848	25.9048785	25.9042753
10		29.0554339	29.0511316	29.0489802	29.0479044	29.0473665
11		32.1974453	32.1935629	32.1916215	32.1906508	32.1901654
12		35.3393825	35.3358453	35.3340765	35.3331921	35.3327498
13		38.4812634	38.4780150	38.4763907	38.4755785	38.4751724
14		41.6231009	41.6200978	41.6185961	41.6178452	41.6174697
15		44.7649041	44.7621117	44.7607154	44.7600173	44.7596682
16		47.9066797	47.9040704	47.9027657	47.9021133	47.9017872
17		51.0484328	51.0459841	51.0447597	51.0441475	51.0438414
18		54.1901673	54.1878606	54.1867072	54.1861304	54.1858421
19		57.3318862	57.3297059	57.3286157	57.3280706	57.3277981
20		60.4735921	60.4715251	60.4704915	60.4699747	60.4697163
21		63.6152868	63.6133218	63.6123393	63.6118481	63.6116024
22		66.7569718	66.7550994	66.7541631	66.7536950	66.7534609
23		69.8986486	69.8968603	69.8959661	69.8955190	69.8952955
24		73.0403181	73.0386068	73.0377510	73.0373232	73.0371092
25		76.1819814	76.1803405	76.1795201	76.1791099	76.1789048
26		79.3236390	79.3220631	79.3212752	79.3208812	79.3206842
27		82.4652916	82.4637758	82.4630179	82.4626390	82.4624495
28		85.6069399	85.6054797	85.6047496	85.6043846	85.6042021
29		88.7485842	88.7471757	88.7464715	88.7461194	88.7459433
30		91.8902250	91.8888647	91.8881845	91.8878444	91.8876744

		alfa i				
delta	128	256	512	1024	2048	
i						
1	.1248780	.0883452	.0624847	.0441888	.0312481	
2	3.8337443	3.8327253	3.8322157	3.8319608	3.8318334	
3	7.0167002	7.0161434	7.0158651	7.0157259	7.0156563	
4	10.1742360	10.1738521	10.1736601	10.1735641	10.1735161	
5	13.3242783	13.3239851	13.3238385	13.3237652	13.3237286	
6	16.4711044	16.4708672	16.4707486	16.4706893	16.4706597	
7	19.6162568	19.6160577	19.6159581	19.6159083	19.6158834	
8	22.7604276	22.7602560	22.7601702	22.7601273	22.7601059	
9	25.9039737	25.9038229	25.9037475	25.9037098	25.9036910	
10	29.0470975	29.0469631	29.0468958	29.0468622	29.0468454	
11	32.1899227	32.1898013	32.1897407	32.1897103	32.1896951	
12	35.3325287	35.3324182	35.3323629	35.3323353	35.3323214	
13	38.4749694	38.4748678	38.4748171	38.4747917	38.4747790	
14	41.6172820	41.6171882	41.6171412	41.6171178	41.6171060	
15	44.7594936	44.7594064	44.7593627	44.7593409	44.7593300	
16	47.9016241	47.9015425	47.9015018	47.9014814	47.9014712	
17	51.0436883	51.0436118	51.0435735	51.0435544	51.0435448	
18	54.1856979	54.1856258	54.1855898	54.1855718	54.1855628	
19	57.3276618	57.3275937	57.3275596	57.3275426	57.3275340	
20	60.4695871	60.4695225	60.4694902	60.4694741	60.4694660	
21	63.6114796	63.6114182	63.6113875	63.6113721	63.6113645	
22	66.7533438	66.7532853	66.7532561	66.7532415	66.7532341	
23	69.8951837	69.8951278	69.8950999	69.8950859	69.8950789	
24	73.0370023	73.0369488	73.0369221	73.0369087	73.0369020	
25	76.1788022	76.1787509	76.1787253	76.1787125	76.1787061	
26	79.3205857	79.3205365	79.3205119	79.3204996	79.3204934	
27	82.4623547	82.4623074	82.4622837	82.4622718	82.4622659	
28	85.6041108	85.6040651	85.6040423	85.6040309	85.6040252	
29	88.7458553	88.7458112	88.7457892	88.7457782	88.7457727	
30	91.8875893	91.8875468	91.8875256	91.8875150	91.8875096	

alfa i					
delta	4096	8192	16384	32768	65536
i					
1	.0220964	.0156248	.0110485	.0078125	.0055243
2	3.8317697	3.8317378	3.8317219	3.8317140	3.8317100
3	7.0156215	7.0156041	7.0155954	7.0155910	7.0155889
4	10.1734921	10.1734801	10.1734741	10.1734711	10.1734696
5	13.3237102	13.3237011	13.3236965	13.3236942	13.3236931
6	16.4706449	16.4706375	16.4706337	16.4706319	16.4706310
7	19.6158710	19.6158648	19.6158616	19.6158601	19.6158593
8	22.7600951	22.7600898	22.7600871	22.7600857	22.7600851
9	25.9036815	25.9036768	25.9036745	25.9036733	25.9036727
10	29.0468370	29.0468328	29.0468307	29.0468296	29.0468291
11	32.1896876	32.1896838	32.1896819	32.1896809	32.1896805
12	35.3323145	35.3323111	35.3323094	35.3323085	35.3323081
13	38.4747727	38.4747695	38.4747679	38.4747671	38.4747667
14	41.6171002	41.6170972	41.6170958	41.6170950	41.6170947
15	44.7593245	44.7593218	44.7593204	44.7593198	44.7593194
16	47.9014661	47.9014635	47.9014622	47.9014616	47.9014613
17	51.0435401	51.0435377	51.0435365	51.0435359	51.0435356
18	54.1855582	54.1855560	54.1855549	54.1855543	54.1855540
19	57.3275298	57.3275277	57.3275266	57.3275261	57.3275258
20	60.4694620	60.4694600	60.4694589	60.4694584	60.4694582
21	63.6113606	63.6113587	63.6113577	63.6113573	63.6113570
22	66.7532305	66.7532287	66.7532277	66.7532273	66.7532270
23	69.8950754	69.8950737	69.8950728	69.8950724	69.8950721
24	73.0368987	73.0368970	73.0368961	73.0368957	73.0368955
25	76.1787029	76.1787013	76.1787005	76.1787001	76.1786999
26	79.3204903	79.3204888	79.3204880	79.3204876	79.3204875
27	82.4622630	82.4622615	82.4622607	82.4622604	82.4622602
28	85.6040224	85.6040209	85.6040202	85.6040199	85.6040197
29	88.7457700	88.7457686	88.7457679	88.7457676	88.7457674
30	91.8875070	91.8875056	91.8875050	91.8875047	91.8875045

	alfa i				
delta	131072	262144	524288	1048576	2097152
i					
1	.0039062	.0027621	.0019531	.0013811	.0009766
2	3.8317080	3.8317070	3.8317065	3.8317062	3.8317061
3	7.0155878	7.0155872	7.0155869	7.0155868	7.0155868
4	10.1734689	10.1734685	10.1734683	10.1734682	10.1734682
5	13.3236925	13.3236922	13.3236921	13.3236920	13.3236920
6	16.4706305	16.4706303	16.4706301	16.4706301	16.4706301
7	19.6158589	19.6158587	19.6158586	19.6158586	19.6158585
8	22.7600847	22.7600846	22.7600845	22.7600844	22.7600844
9	25.9036724	25.9036723	25.9036722	25.9036722	25.9036721
10	29.0468288	29.0468287	29.0468287	29.0468286	29.0468286
11	32.1896802	32.1896801	32.1896800	32.1896800	32.1896800
12	35.3323078	35.3323077	35.3323077	35.3323077	35.3323076
13	38.4747665	38.4747664	38.4747664	38.4747663	38.4747663
14	41.6170945	41.6170944	41.6170943	41.6170943	41.6170943
15	44.7593193	44.7593192	44.7593191	44.7593191	44.7593191
16	47.9014611	47.9014611	47.9014610	47.9014610	47.9014610
17	51.0435354	51.0435353	51.0435353	51.0435353	51.0435353
18	54.1855539	54.1855538	54.1855538	54.1855537	54.1855537
19	57.3275256	57.3275256	57.3275256	57.3275255	57.3275255
20	60.4694581	60.4694580	60.4694580	60.4694580	60.4694579
21	63.6113569	63.6113569	63.6113568	63.6113568	63.6113568
22	66.7532269	66.7532269	66.7532268	66.7532268	66.7532268
23	69.8950720	69.8950720	69.8950720	69.8950719	69.8950719
24	73.0368954	73.0368954	73.0368953	73.0368953	73.0368953
25	76.1786998	76.1786997	76.1786997	76.1786997	76.1786997
26	79.3204873	79.3204873	79.3204873	79.3204873	79.3204873
27	82.4622601	82.4622600	82.4622600	82.4622600	82.4622600
28	85.6040196	85.6040195	85.6040195	85.6040195	85.6040195
29	88.7457673	88.7457673	88.7457672	88.7457672	88.7457672
30	91.8875044	91.8875044	91.8875043	91.8875043	91.8875043

alfa i					
delta	4194304	8388608	16777216	33554432	67108864
i					
1	.0006905	.0004883	.0003453	.0002441	.0001726
2	3.8317060	3.8317060	3.8317060	3.8317060	3.8317060
3	7.0155867	7.0155867	7.0155867	7.0155867	7.0155867
4	10.1734681	10.1734681	10.1734681	10.1734681	10.1734681
5	13.3236919	13.3236919	13.3236919	13.3236919	13.3236919
6	16.4706300	16.4706300	16.4706300	16.4706300	16.4706300
7	19.6158585	19.6158585	19.6158585	19.6158585	19.6158585
8	22.7600844	22.7600844	22.7600844	22.7600844	22.7600844
9	25.9036721	25.9036721	25.9036721	25.9036721	25.9036721
10	29.0468286	29.0468286	29.0468286	29.0468286	29.0468286
11	32.1896800	32.1896800	32.1896800	32.1896800	32.1896800
12	35.3323076	35.3323076	35.3323076	35.3323076	35.3323076
13	38.4747663	38.4747663	38.4747663	38.4747663	38.4747663
14	41.6170943	41.6170943	41.6170943	41.6170943	41.6170943
15	44.7593191	44.7593191	44.7593191	44.7593191	44.7593191
16	47.9014610	47.9014610	47.9014610	47.9014610	47.9014610
17	51.0435353	51.0435353	51.0435353	51.0435353	51.0435353
18	54.1855537	54.1855537	54.1855537	54.1855537	54.1855537
19	57.3275255	57.3275255	57.3275255	57.3275255	57.3275255
20	60.4694579	60.4694579	60.4694579	60.4694579	60.4694579
21	63.6113568	63.6113568	63.6113568	63.6113568	63.6113568
22	66.7532268	66.7532268	66.7532268	66.7532268	66.7532268
23	69.8950719	69.8950719	69.8950719	69.8950719	69.8950719
24	73.0368953	73.0368953	73.0368953	73.0368953	73.0368953
25	76.1786997	76.1786997	76.1786997	76.1786997	76.1786997
26	79.3204873	79.3204873	79.3204873	79.3204873	79.3204873
27	82.4622600	82.4622600	82.4622600	82.4622600	82.4622600
28	85.6040195	85.6040195	85.6040195	85.6040195	85.6040195
29	88.7457672	88.7457672	88.7457672	88.7457672	88.7457672
30	91.8875043	91.8875043	91.8875043	91.8875043	91.8875043

delta	beta i				
	.125	.250	.500	1	2
i					
1	1.5525781	1.4697956	1.3383772	1.2070921	1.1142546
2	-.9162988	-.7278092	-.4922691	-.2901494	-.1571596
3	.6189424	.4183493	.2421773	.1289081	.0661898
4	-.4430213	-.2699274	-.1464150	-.0755689	-.0382776
5	.3316160	.1898056	.0998464	.0508804	.0256352
6	-.2576606	-.1419066	-.0734361	-.0371831	-.0186852
7	.2064453	.1109217	.0568498	.0286801	.0143910
8	-.1696211	-.0896358	-.0456594	-.0229825	-.0115216
9	.1422699	.0743162	.0377001	.0189476	.0094932
10	-.1213828	-.0628776	-.0318051	-.0159681	-.0079970
11	.1050498	.0540799	.0272973	.0136945	.0068563
12	-.0920165	-.0471468	-.0237601	-.0119132	-.0059632
13	.0814334	.0415710	.0209246	.0104869	.0052483
14	-.0727089	-.0370092	-.0186105	-.0093240	-.0046657
15	.0654212	.0332216	.0166931	.0083611	.0041834
16	-.0592628	-.0300367	-.0150834	-.0075532	-.0037788
17	.0540051	.0273286	.0137165	.0068674	.0034355
18	-.0494754	-.0250033	-.0125440	-.0062795	-.0031412
19	.0455410	.0229892	.0115294	.0057708	.0028866
20	-.0420985	-.0212312	-.0106445	-.0053274	-.0026647
21	.0390664	.0196860	.0098672	.0049379	.0024698
22	-.0363797	-.0183191	-.0091801	-.0045936	-.0022975
23	.0339859	.0171032	.0085691	.0042876	.0021444
24	-.0318425	-.0160159	-.0080229	-.0040141	-.0020076
25	.0299143	.0150390	.0075324	.0037685	.0018847
26	-.0281725	-.0141574	-.0070899	-.0035469	-.0017739
27	.0265928	.0133585	.0066891	.0033463	.0016735
28	-.0251549	-.0126320	-.0063246	-.0031638	-.0015822
29	.0238417	.0119690	.0059921	.0029974	.0014989
30	-.0226386	-.0113620	-.0056877	-.0028450	-.0014227

delta	beta i				
	4	8	16	32	64
i					
1	1.0598419	1.0305914	1.0154612	1.0077717	1.0038960
2	-.0816082	-.0415484	-.0209576	-.0105242	-.0052734
3	.0334883	.0168366	.0084406	.0042258	.0021142
4	-.0192478	-.0096493	-.0048307	-.0024169	-.0012088
5	.0128603	.0064400	.0032224	.0016118	.0008060
6	-.0093630	-.0046862	-.0023442	-.0011724	-.0005863
7	.0072066	.0036059	.0018035	.0009019	.0004510
8	-.0057674	-.0028852	-.0014430	-.0007216	-.0003608
9	.0047508	.0023764	.0011884	.0005943	.0002971
10	-.0040013	-.0020013	-.0010008	-.0005004	-.0002502
11	.0034301	.0017155	.0008579	.0004290	.0002145
12	-.0029830	-.0014918	-.0007460	-.0003730	-.0001865
13	.0026252	.0013129	.0006565	.0003283	.0001641
14	-.0023337	-.0011670	-.0005836	-.0002918	-.0001459
15	.0020923	.0010463	.0005232	.0002616	.0001308
16	-.0018899	-.0009451	-.0004726	-.0002363	-.0001181
17	.0017182	.0008592	.0004296	.0002148	.0001074
18	-.0015709	-.0007855	-.0003928	-.0001964	-.0000982
19	.0014436	.0007218	.0003609	.0001805	.0000902
20	-.0013326	-.0006663	-.0003332	-.0001666	-.0000833
21	.0012351	.0006176	.0003088	.0001544	.0000772
22	-.0011489	-.0005745	-.0002873	-.0001436	-.0000718
23	.0010723	.0005362	.0002681	.0001341	.0000670
24	-.0010039	-.0005020	-.0002510	-.0001255	-.0000627
25	.0009424	.0004712	.0002356	.0001178	.0000589
26	-.0008870	-.0004435	-.0002218	-.0001109	-.0000554
27	.0008368	.0004184	.0002092	.0001046	.0000523
28	-.0007912	-.0003956	-.0001978	-.0000989	-.0000494
29	.0007495	.0003748	.0001874	.0000937	.0000468
30	-.0007114	-.0003557	-.0001779	-.0000889	-.0000445

		beta i				
delta	128	256	512	1024	2048	
i						
1	1.0019507	1.0009759	1.0004878	1.0002445	1.0001211	
2	-.0026395	-.0013205	-.0006604	-.0003303	-.0001651	
3	.0010575	.0005288	.0002644	.0001322	.0000661	
4	-.0006045	-.0003023	-.0001511	-.0000756	-.0000378	
5	.0004031	.0002015	.0001008	.0000504	.0000252	
6	-.0002931	-.0001466	-.0000733	-.0000366	-.0000183	
7	.0002255	.0001128	.0000564	.0000282	.0000141	
8	-.0001804	-.0000902	-.0000451	-.0000225	-.0000113	
9	.0001486	.0000743	.0000371	.0000186	.0000093	
10	-.0001251	-.0000626	-.0000313	-.0000156	-.0000078	
11	.0001072	.0000536	.0000268	.0000134	.0000067	
12	-.0000933	-.0000466	-.0000233	-.0000117	-.0000058	
13	.0000821	.0000410	.0000205	.0000103	.0000051	
14	-.0000729	-.0000365	-.0000182	-.0000091	-.0000046	
15	.0000654	.0000327	.0000163	.0000082	.0000041	
16	-.0000591	-.0000295	-.0000148	-.0000074	-.0000037	
17	.0000537	.0000268	.0000134	.0000067	.0000034	
18	-.0000491	-.0000245	-.0000123	-.0000061	-.0000031	
19	.0000451	.0000226	.0000113	.0000056	.0000028	
20	-.0000416	-.0000208	-.0000104	-.0000052	-.0000026	
21	.0000386	.0000193	.0000097	.0000048	.0000024	
22	-.0000359	-.0000180	-.0000090	-.0000045	-.0000022	
23	.0000335	.0000168	.0000084	.0000042	.0000021	
24	-.0000314	-.0000157	-.0000078	-.0000039	-.0000020	
25	.0000295	.0000147	.0000074	.0000037	.0000018	
26	-.0000277	-.0000139	-.0000069	-.0000035	-.0000017	
27	.0000262	.0000131	.0000065	.0000033	.0000016	
28	-.0000247	-.0000124	-.0000062	-.0000031	-.0000015	
29	.0000234	.0000117	.0000059	.0000029	.0000015	
30	-.0000222	-.0000111	-.0000056	-.0000028	-.0000014	

beta i					
delta	4096	8192	16384	32768	65536
i					
1	1.0000601	1.0000286	1.0000155	1.0000038	1.0000081
2	-.0000826	-.0000413	-.0000206	-.0000103	-.0000052
3	.0000331	.0000165	.0000083	.0000041	.0000021
4	-.0000189	-.0000094	-.0000047	-.0000024	-.0000012
5	.0000126	.0000063	.0000031	.0000016	.0000008
6	-.0000092	-.0000046	-.0000023	-.0000011	-.0000006
7	.0000071	.0000035	.0000018	.0000009	.0000004
8	-.0000056	-.0000028	-.0000014	-.0000007	-.0000004
9	.0000046	.0000023	.0000012	.0000006	.0000003
10	-.0000039	-.0000020	-.0000010	-.0000005	-.0000002
11	.0000034	.0000017	.0000008	.0000004	.0000002
12	-.0000029	-.0000015	-.0000007	-.0000004	-.0000002
13	.0000026	.0000013	.0000006	.0000003	.0000002
14	-.0000023	-.0000011	-.0000006	-.0000003	-.0000001
15	.0000020	.0000010	.0000005	.0000003	.0000001
16	-.0000018	-.0000009	-.0000005	-.0000002	-.0000001
17	.0000017	.0000008	.0000004	.0000002	.0000001
18	-.0000015	-.0000008	-.0000004	-.0000002	-.0000001
19	.0000014	.0000007	.0000004	.0000002	.0000001
20	-.0000013	-.0000007	-.0000003	-.0000002	-.0000001
21	.0000012	.0000006	.0000003	.0000002	.0000001
22	-.0000011	-.0000006	-.0000003	-.0000001	-.0000001
23	.0000010	.0000005	.0000003	.0000001	.0000001
24	-.0000010	-.0000005	-.0000002	-.0000001	-.0000001
25	.0000009	.0000005	.0000002	.0000001	.0000001
26	-.0000009	-.0000004	-.0000002	-.0000001	-.0000001
27	.0000008	.0000004	.0000002	.0000001	.0000001
28	-.0000008	-.0000004	-.0000002	-.0000001	-.0000001
29	.0000007	.0000004	.0000002	.0000001	.0000000
30	-.0000007	-.0000003	-.0000002	-.0000001	.0000000

		beta i				
delta	131072	262144	524288	1048576	2097152	
i						
1	1.0000057	1.0000055	1.0000148	1.0000170	1.0000304	
2	-.0000026	-.0000013	-.0000006	-.0000003	-.0000002	
3	.0000010	.0000005	.0000003	.0000001	.0000001	
4	-.0000006	-.0000003	-.0000002	-.0000001	.0000000	
5	.0000004	.0000002	.0000001	.0000000	.0000000	
6	-.0000003	-.0000001	-.0000001	.0000000	.0000000	
7	.0000002	.0000001	.0000001	.0000000	.0000000	
8	-.0000002	-.0000001	.0000000	.0000000	.0000000	
9	.0000001	.0000001	.0000000	.0000000	.0000000	
10	-.0000001	-.0000001	.0000000	.0000000	.0000000	
11	.0000001	.0000001	.0000000	.0000000	.0000000	
12	-.0000001	.0000000	.0000000	.0000000	.0000000	
13	.0000001	.0000000	.0000000	.0000000	.0000000	
14	-.0000001	.0000000	.0000000	.0000000	.0000000	
15	.0000001	.0000000	.0000000	.0000000	.0000000	
16	-.0000001	.0000000	.0000000	.0000000	.0000000	
17	.0000001	.0000000	.0000000	.0000000	.0000000	
18	.0000000	.0000000	.0000000	.0000000	.0000000	
19	.0000000	.0000000	.0000000	.0000000	.0000000	
20	.0000000	.0000000	.0000000	.0000000	.0000000	
21	.0000000	.0000000	.0000000	.0000000	.0000000	
22	.0000000	.0000000	.0000000	.0000000	.0000000	
23	.0000000	.0000000	.0000000	.0000000	.0000000	
24	.0000000	.0000000	.0000000	.0000000	.0000000	
25	.0000000	.0000000	.0000000	.0000000	.0000000	
26	.0000000	.0000000	.0000000	.0000000	.0000000	
27	.0000000	.0000000	.0000000	.0000000	.0000000	
28	.0000000	.0000000	.0000000	.0000000	.0000000	
29	.0000000	.0000000	.0000000	.0000000	.0000000	
30	.0000000	.0000000	.0000000	.0000000	.0000000	

	beta i				
delta	4194304	8388608	16777216	33554432	67108864
i					
1	1.0000388	1.0000000	1.0000000	1.0000000	1.0000000
2	-.0000001	.0000000	.0000000	.0000000	.0000000
3	.0000000	.0000000	.0000000	.0000001	.0000000
4	.0000000	.0000000	.0000000	.0000000	.0000000
5	.0000000	.0000000	.0000000	.0000000	.0000000
6	.0000000	.0000000	.0000000	.0000000	.0000000
7	.0000000	.0000000	.0000000	.0000000	.0000000
8	.0000000	.0000000	.0000000	.0000000	.0000000
9	.0000000	.0000000	.0000000	.0000000	.0000000
10	.0000000	.0000000	.0000000	.0000000	.0000000
11	.0000000	.0000000	.0000000	.0000000	.0000000
12	.0000000	.0000000	.0000000	.0000000	.0000000
13	.0000000	.0000000	.0000000	.0000000	.0000000
14	.0000000	.0000000	.0000000	.0000000	.0000000
15	.0000000	.0000000	.0000000	.0000000	.0000000
16	.0000000	.0000000	.0000000	.0000000	.0000000
17	.0000000	.0000000	.0000000	.0000000	.0000000
18	.0000000	.0000000	.0000000	.0000000	.0000000
19	.0000000	.0000000	.0000000	.0000000	.0000000
20	.0000000	.0000000	.0000000	.0000000	.0000000
21	.0000000	.0000000	.0000000	.0000000	.0000000
22	.0000000	.0000000	.0000000	.0000000	.0000000
23	.0000000	.0000000	.0000000	.0000000	.0000000
24	.0000000	.0000000	.0000000	.0000000	.0000000
25	.0000000	.0000000	.0000000	.0000000	.0000000
26	.0000000	.0000000	.0000000	.0000000	.0000000
27	.0000000	.0000000	.0000000	.0000000	.0000000
28	.0000000	.0000000	.0000000	.0000000	.0000000
29	.0000000	.0000000	.0000000	.0000000	.0000000
30	.0000000	.0000000	.0000000	.0000000	.0000000

begin

integer k,n,i,j,v,s,z,l;
real eps,sgm,R,h,Eo,xb,Et,ga,gb,Q,sigma,w,dt,a,b,c,d,bt,
xx,ya,yb,T,Tr,omega,gamma,da,y1,R1,gm1,gmp,dt1,dtp,
b1,ua,ub,uc,cst;

array alfa,wa[1:30,1:30],alf,war[1:30];

read(alfa,wa);

wait('dane');

read(k,n,eps,sgm,R);

begin

integer array m[1:n];

array p,temp,ss,st,af[1:n];

read(m,p,temp);

v:=0;

for i:=1 step 1 until n do v:=v+m[i];

begin

array X,E,delta[1:v],WW[1:4],WN1,WN2,WN3,WN4,WN5,WN6[1:7];

switch TE=QA,QB,QC,QD,QE,QF;

real procedure F(x);

value x;

real x;

begin

real p;

integer i;

p:=0;

```

    for i:=1 step 1 until 4 do p:=p*x+WW[i];
    F:=p*x
  end F;
real procedure CONC(x,delta);
  value x,delta;
  real x,delta;
  begin
    real a,s,t;
    s:=(1/dtp+sqrt(2/delta));
    t:=(1/dtp-sqrt(2/delta))*exp(-sqrt(8/delta)*(da+x));
    a:=sqrt(2/delta)*(s+t)/((s-t)*R);
    s:=(a+b1)/(a-b1);
    CONC:=(s-1)/(s*exp(b1*y1)-exp(-b1*y1))
  end CONC;
real procedure BESSEL(n,x);
  value n,x;
  integer n;
  real x;
  begin
    integer i;
    real p,w,f;
    w:=0;
    if n=0 then go to EA;
    go to if x>3 then ED else EC;
  EA:if x>3 then go to EB;

```

```

    p:=x*x/9;
    for i:=1 step 1 until 7 do
        w:=w*p+WN1[i];
    go to FINISH;
EB:f:=0;
    p:=3/x;
    for i:=1 step 1 until 7 do
        begin
            f:=f*p+WN2[i];
            w:=w*p+WN3[i]
        end;
    w:=f*cos(w+x)/sqrt(x);
    go to FINISH;
EC:p:=x*x/9;
    for i:=1 step 1 until 7 do
        w:=w*p+WN4[i];
    w:=w*x;
    go to FINISH;
ED:f:=0;
    p:=3/x;
    for i:=1 step 1 until 7 do
        begin
            f:=f*p+WN5[i];
            w:=w*p+WN6[i]
        end;

```

$$w=f \times \cos(w+x) / \text{sqrt}(x);$$

FINISH: BESSEL=w

end BESSEL;

WN1 [1]= 0.0002100;
WN1 [2]=-0.0039444;
WN1 [3]= 0.0444479;
WN1 [4]=-0.3163866;
WN1 [5]= 1.2656208;
WN1 [6]=-2.2499997;
WN1 [7]= 1;
WN2 [1]= 0.00014476;
WN2 [2]=-0.00072805;
WN2 [3]= 0.00137237;
WN2 [4]=-0.00009512;
WN2 [5]=-0.00552740;
WN2 [6]=-0.00000077;
WN2 [7]= 0.79788456;
WN3 [1]= 0.00013558;
WN3 [2]=-0.00029333;
WN3 [3]=-0.00054125;
WN3 [4]= 0.00262573;
WN3 [5]=-0.00003954;
WN3 [6]=-0.04166397;
WN3 [7]=-0.78539816;
WN4 [1]= 0.00001109;

WN4[2]:=-0.00031761;
WN4[3]= 0.00443319;
WN4[4]:=-0.03954289;
WN4[5]= 0.21093573;
WN4[6]:=-0.56249985;
WN4[7]= 0.5;
WN5[1]:=-0.00020033;
WN5[2]= 0.00113653;
WN5[3]:=-0.00249511;
WN5[4]= 0.00017105;
WN5[5]= 0.01659667;
WN5[6]= 0.00000156;
WN5[7]= 0.79788456;
WN6[1]:=-0.00029166;
WN6[2]= 0.00079824;
WN6[3]= 0.00074348;
WN6[4]:=-0.00637879;
WN6[5]= 0.00005650;
WN6[6]= 0.12499612;
WN6[7]:=-2.35619449;
WW[1]= 1.48098339₁₀⁻¹¹;
WW[2]:=-3.60121584₁₀⁻⁸;
WW[3]= 4.62395134₁₀⁻⁵;
WW[4]= 3.85014117₁₀⁻²;
da:=30;

```

y1=30;
R1=1.75;
gm1=110-4;
gmp=110-4;
read(X,E); h=0.5; v=0;
for i=1 step 1 until n do
  begin
    Eo=F(temp[i]);
    for j=1 step 1 until m[i] do
      begin
        xb=0;
        Et=Eo+E[v+j]/100;
        if Et=0 then go to ZD;
        if Et<0 then h=-abs(h) else h=abs(h);
        if F(xb) -Et<0 then go to ZB;
        ZA:if F(xb) -Et>0 then
          begin
            xb=xb+h; go to ZA
          end;
          ga=xb; gb=xb-h; go to ZC;
        ZB:if F(xb) -Et<0 then
          begin
            xb=xb+h; go to ZB
          end;
          gb=xb; ga=xb-h;

```

```

    ZC:xb=(ga+gb)/2;
    if F(xb) -Et>0 then gb:=xb else ga:=xb;
    if abs(ga-gb)>10-8 then go to ZC;
    ZD:delta[v+j]:=xb-temp[i]
    end;
    v:=v+m[i]
end;
v:=0;
for i=1 step 1 until n do st[i]:=0;
for i=1 step 1 until n do
    begin
        a:=b:=c:=d:=0;
        for j=1 step 1 until m[i] do
            begin
                a:=a+X[v+j];
                b:=b+ln(delta[v+j]);
                c:=c+X[v+j]*X[v+j];
                d:=d+X[v+j]*ln(delta[v+j])
            end;
        xb:=m[i]*c-a*a;
        af[i]=(m[i]*d-a*b)/xb;
        bt:=(b*c-a*d)/xb;
        xb:=exp(bt+af[i]*X[v+1]);
        for j=2 step 1 until m[i]-1 do
            begin

```

```

        delta[v+j]:=delta[v+j]/xb;
        X[v+j]:=X[v+1]-X[v+j];
        st[i]:=st[i]+(ln(delta[v+j])+af[i]*X[v+j])t2
    end;
    v:=v+m[i]
end;
line(1);
print('Experiment no. '); format('11'); print(k);
line(2);
print('No. of molecules present at temperature 1000/T ln(gamma)
[degK] [torr] Present Smith-Linnett
analysis analysis');
format(' ?11 11.1 11 1.11 1.1110-1 1.1110-1 1.11 1.1110-1 ');
line(1);
v:=0;
for i:=1 step 1 until n do
    begin
        T:=temp[i]+273;
        Tr=T/eps;
        omega:=1.075*exp(-0.1615*ln(Tr));
        omega:=omega+2*exp(-0.3213779166*ln(10*Tr)*ln(10*Tr));
        dt1:=0.4756087837*T/(gm1*R1*p[i]*sgm*sgm*omega);
        dtp:=0.4756087837*T/(gmp*R*p[i]*sgm*sgm*omega);
        b1:=sqrt(2/dt1)/R1;
        go to P;
    end;

```



```

LA:Q:=0;
  cst:=CONC(0.0,0.125*2↑(1-1));
  for j:=2 step 1 until m[i]-1 do
    begin
      sigma:=0;
      s:=1;
      CA:ua:=alfa[1,s]*dtp+1;
      ub:=exp(-2*alfa[1,s]*da/R);
      uc:=exp(-alfa[1,s]*X[v+j]/R);
      w:=wa[1,s]*(ua+(ua-2)*ub)*uc/(ua+(ua-2)*ub*uc*uc);
      s:=s+1;
      sigma:=sigma+w;
      if abs(w)>110-8 then go to CA;
      sigma:=CONC(X[v+j],0.125*2↑(1-1))*sigma/cst;
      Q:=Q+(ln(delta[v+j])-ln(sigma))↑2
    end;
  go to TE[z];
LB:sigma:=xb:=0;
  j:=1;
  cst:=CONC(0.0,dt);
AB:if BESSEL(0,xb)<dt*xb*BESSEL(1,xb) then go to YB;
YA:if BESSEL(0,xb)>dt*xb*BESSEL(1,xb) then
  begin
    xb:=xb+1;
    go to YA
  
```

```

    end;
    ga:=xb; gb:=xb-1; go to YC;
YB:if BESSEL(0,xb)<dt*xb*BESSEL(1,xb) then
    begin
        xb:=xb+1;
        go to YB
    end;
    gb:=xb; ga:=xb-1;
YC:xb:=(ga+gb)/2;
    if BESSEL(0,xb)>dt*xb*BESSEL(1,xb) then gb:=xb
        else ga:=xb;

    if abs(ga-gb)>110-8 then go to YC;
    alf[j]:=xb;
    war[j]:=2/(xb*(1+xb*xb*dt*dt)*BESSEL(1,xb));
    ua:=alf[j]*dtp+1;
    ub:=exp(-2*alf[j]*da/R);
    uc:=exp(-alf[j]*X[v+m[i]-1]/R);
    w:=war[j]*(ua+(ua-2)*ub)*uc/(ua+(ua-2)*ub*uc*uc);
    sigma:=sigma+w;
    j:=j+1;
    xb:=xb+1;
    if abs(w)>110-8 then go to AB;
    sigma:=CONC(X[v+m[i]-1],dt)*sigma/cst;
    Q:=(ln(delta[v+m[i]-1])-ln(sigma))*t2;
    for j:=2 step 1 until m[i]-2 do

```

```

begin
  sigma:=0;
  s=1;
  DA:ua:=alf[s]*dtp+1;
  ub:=exp(-2*alf[s]*da/R);
  uc:=exp(-alf[s]*X[v+j]/R);
  w=war[s]*(ua+(ua-2)*ub)*uc/(ua+(ua-2)*ub*uc*uc);
  s=s+1;
  sigma=sigma+w;
  if abs(w)>110-8 then go to DA;
  sigma=CONC(X[v+j],dt)*sigma/cst;
  Q:=Q+(ln(delta[v+j])-ln(sigma))*t2
end;
  go to TE[z];
  P:xx=0.125;
  l:=1;
  z:=1;
  go to LA;
  QA:a:=Q;
  l:=2;
  z:=2;
  go to LA;
  QB:b:=Q;
  l:=3;
  z:=3;

```

```

    go to LA;
QC: c:=Q;
    if a>b^c>b then go to XC;
    xx=2*xx;
    l=l+1;
    a=b;
    b=c;
    go to LA;
XC: h=xx;
    dt=3*xx;
    z=4;
    go to LB;
QD: ya=Q;
    if a>b^ya>b then
        begin
            c=ya;
            go to XB
        end;
    xx=xx+h;
    a=b;
    b=ya;
XB: if 2*h<1n-8 then go to SOL;
    h=h/2;
    dt=xx+h;
    z=5;

```

```

    go to LB;
QE:ya:=Q;
    if a>ya^b>ya then
        begin
            c:=b;
            b:=ya;
            go to XB
        end;
    dt:=xx+3×h;
    z:=6;
    go to LB;
QF:yb:=Q;
    if ya>b^yb>b then
        begin
            xx=xx+h;
            a:=ya;
            c:=yb;
            go to XB
        end;
    xx=xx+2×h;
    a=b;
    b=yb;
    go to XB;
SOL:xx=xx+h;
    gamma:=0.4756087837×T/(xx×R<p[i]>×sgm×sgm×omega);

```

```

w:=2/(af[i]*af[i]*R*R);
w:=0.4756087837*T/(w*R*p[i]*sgn*sgn*omega);
print(i,T,p[i]/1000,gamma,w,1000/T,ln(gamma));
ss[i]:=b;
v:=v+m[i]
    end;
line(15);
print('Experiment now'); format('11');
print(k); line(1);
print('~~~~Sum of the least squares
No~~~~one dim~~~~three dim
~~~~equation~~~~equation');
format(' ?11~~~~1.11110-11~~~~1.11110-11');
line(1);
for i=1 step 1 until n do print(i,st[i],ss[i]);
line(15)
    end
end
end?

```

Biblioteka Instytutu Chemii Fizycznej PAN

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