LEUNA WORKS, DECEMBER 17, 1941

CALCULATION OF THE EQUILIBRIUM FOR THE DEHYDROGENATION OF BUTANE

The equilibrium constants and the position of the equilibrium have been calculated from the literature data available.

The following three reactions must be distinguished in the dehydrogenation of n-butane:

1) dehydrogenation to butene -1

2) " " butene -2 (trans)

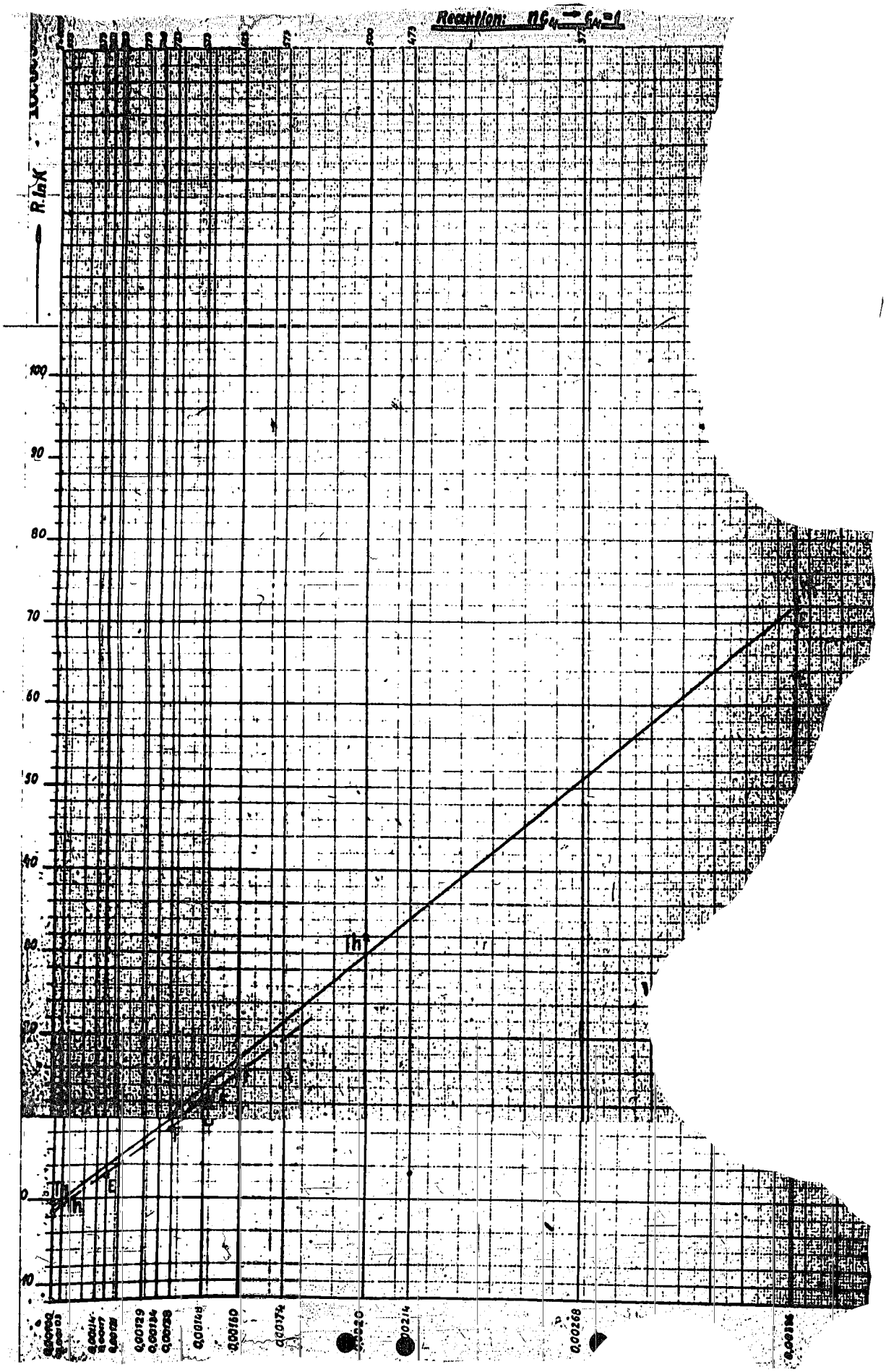
3) " " butene -2 (cis)

Isobutane always gives isobutylene on dehydrogenation. The free energy data given in Volume II of Ellis, "The Chemistry of Petroleum Derivatives" have been used.

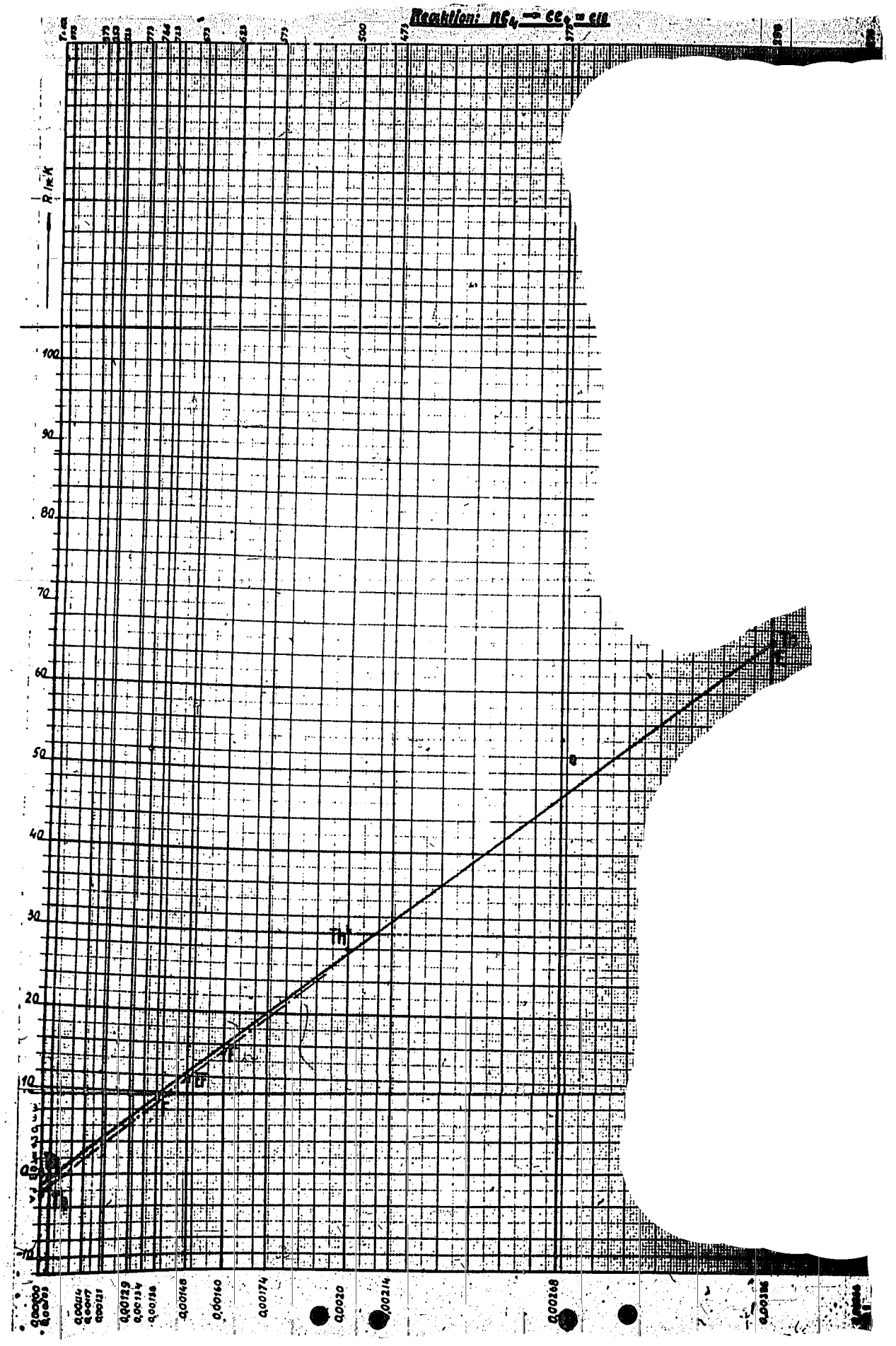
Furthermore, the data of Frey and Huppke, Ind. Eng. Chem. 25, 35 and Thomas, Egloff and Morell, Ind. Eng. Chem. 29, 1620, have been used. The points calculated from the data of Ellis are marked with E on the diagrams whereas the values from Frey and Huppke are marked F and the values from Thomas are marked Th. In the attached diagrams the values for $-RlnK$ are plotted against $\frac{1}{T}$ for the four reactions mentioned above.

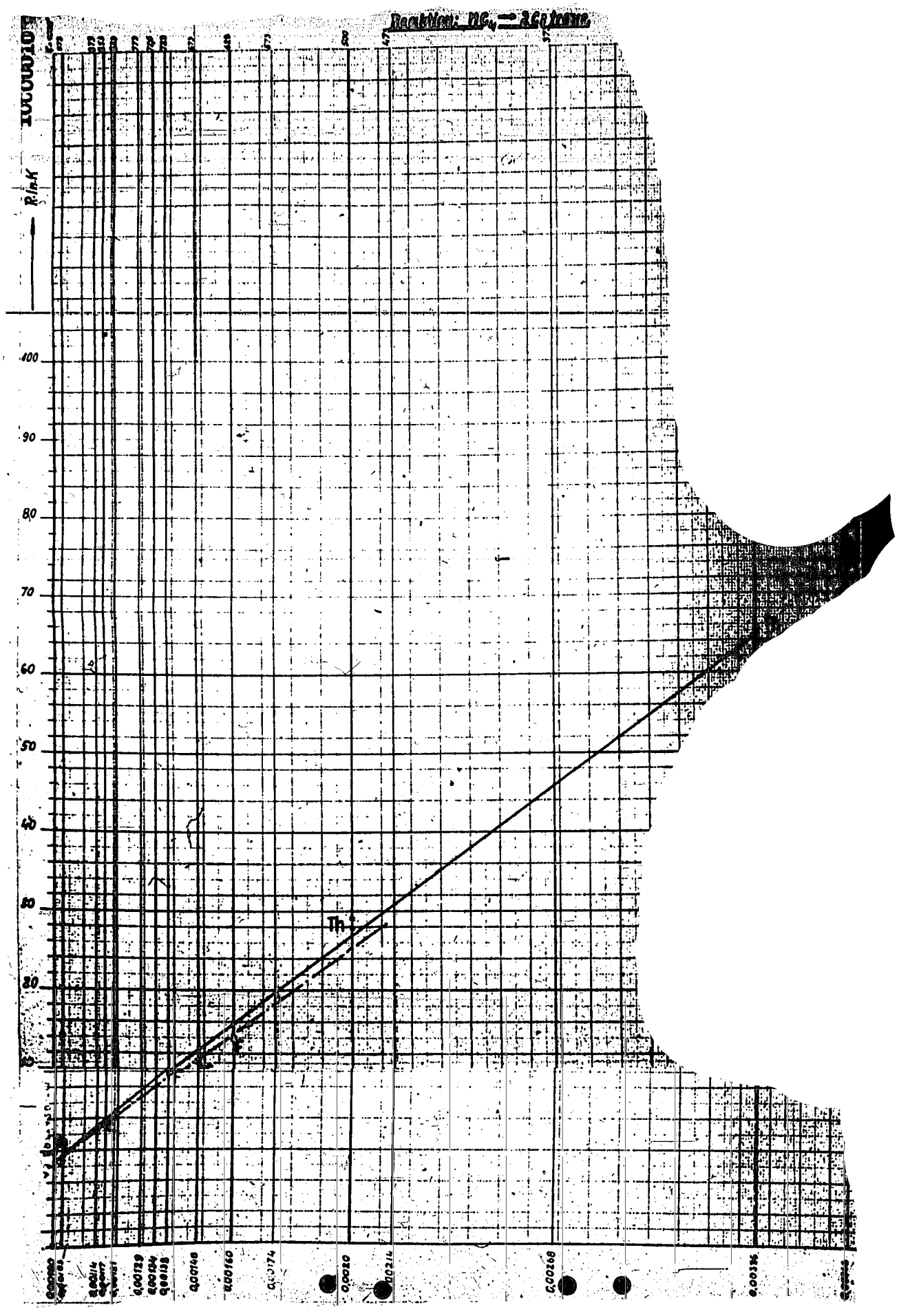
The following table gives the equilibrium constants for the temperatures of 1022°F. and 1076°F. which were obtained by interpolation between the calculated values. The table also shows the equilibrium concentrations of the olefins in percentages. The calculations are based on the assumption that the total pressure is 1 atm. and the gas is composed entirely of n- or isobutane.

Olefin Formed	Temperature °F.	K (kg cm^{-2})	Concentration of butylene %
butene -1	1022	0.0989	23
	1076	0.180	28
isobutylene	1022	0.494	35
	1076	0.904	41
butene -2 (trans)	1022	0.134	26
	1076	0.220	30
butene -2 (cis)	1022	0.144	26
	1076	0.245	31



Reaktion: $nC_4 \rightarrow C_4 = 1$
R.lnK
100
90
80
70
60
50
40
30
20
10
0
Th
E
0,00160
0,00174
0,00214
0,00268


Reaktion: nC4 → cC4 = cB
R ln K
100
90
80
70
60
50
40
30
20
10
0
-10
Th
0,00100
0,00114
0,00117
0,00121
0,00129
0,00134
0,00138
0,00148
0,00160
0,00174
0,0020
0,00214
0,00268
0,00386



Reaktion: $NC_4 \rightarrow 2C_2$ [illegible]
R.lnK
100
90
80
70
60
50
40
30
20
10
Th
0,00120
0,00114
0,00129
0,00104
0,00138
0,00148
0,00160
0,00174
0,0020
0,00214
0,00268
0,00336