

# ВЫЧИСЛЕНИЕ БАЗОВЫХ ВЕЩЕСТВ В ГРУППАХ ЭЛЕМЕНТОВ

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**Аннотация:** составляется список базовых реакций в группе заданных элементов и веществ по разработанной программе. В список включаются все реакции, которые могут быть составлены по материальному балансу элементов веществ для каждой реакции. Из списка выбираются группы линейно независимых реакций, формируется новый список групп линейно независимых реакций. Из нового списка выбирается группа, обладающая наибольшим суммарным термодинамическим потенциалом, отнесенным к единице суммарной массы. В итоге получается некоторая реакция, обладающая линейно независимыми свойствами с наличием всех заданных веществ.

**Ключевые слова:** группа элементов, группа веществ, все реакции, линейно независимые реакции, группа с максимальным потенциалом.

## CALCULATION OF BASE SUBSTANCES IN GROUPS OF ELEMENTS

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**Abstract:** a list of basic reactions in a group of given elements and substances is compiled according to the developed program. The list includes all reactions that can be compiled according to the material balance of the elements of substances for each reaction. Groups of linearly independent reactions are selected from the list, a new list of groups of linearly independent reactions is formed. From the new list, a group is selected that has the highest total thermodynamic potential per unit of total mass. As a result, some reaction is obtained that has linearly independent properties with the presence of all given substances.

**Keywords:** group of elements, group of substances, all reactions, linearly independent reactions, group with maximum potential.

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Составляется список базовых реакций в группе заданных элементов и веществ по разработанной программе. В список включаются все реакции, которые могут быть составлены по материальному балансу элементов веществ для каждой реакции. Из списка выбираются группы линейно независимых реакций, формируется новый список групп линейно независимых реакций. Из нового списка выбирается группа, обладающая наибольшим суммарным термодинамическим потенциалом, отнесенным к единице суммарной массы. В итоге получается некоторая реакция, обладающая линейно независимыми свойствами с наличием всех заданных веществ.

### Группа элементов С-Н-О

#### Начальные данные

$n_b = 3$   $n_p = 12$   $t_k = 1000$  К

Атомные веса элементов:

12.00 1.01 16.00

Наименования веществ  $dh_f$ , ккал/моль  $s_0$ , кал/мольК

С	0.000	1.372
O2	0.000	49.005
CH4	-17.880	44.530
C2H2	54.020	48.000
C2H6	-20.250	54.850
C3H4	45.920	58.300
C4H6	34.970	67.710
C4H10	-30.150	74.120
C5H12	-36.920	82.120
C6H12	-29.430	71.280
C7H16	44.880	102.270
H2O	-57.796	45.106

Матрица групп элементов в веществах

1.0 0.0 0.0  
0.0 0.0 2.0

1.0 4.0 0.0  
2.0 2.0 0.0  
2.0 6.0 0.0  
3.0 4.0 0.0  
4.0 6.0 0.0  
4.0 10.0 0.0  
5.0 12.0 0.0  
6.0 12.0 0.0  
7.0 16.0 0.0  
0.0 2.0 1.0

Расчетные данные

1)  $3C5H12 + 1C6H12 = 3C7H16$  135 318 -140 307  
(sSfp-sSfl)=-1.08300000000745E+0001 T0s= -25377  
t0= -25377

2)  $2C4H10 + 1C6H12 = 2C7H16$  90 220 -90 205  
(sSfp-sSfl)=-1.49799999999814E+0001 T0s= -11982  
t0= -11982

3)  $6C4H6 + 6C7H16 = 11C6H12$  -324 1020 479 784  
(sSfp-sSfl)=-2.35799999999814E+0002 T0s= 3405  
t0= 3405

4)  $3C3H4 + 3C7H16 = 5C6H12$  -147 482 272 356  
(sSfp-sSfl)=-1.25309999999590E+0002 T0s= 3348  
t0= 3348

5)  $6C2H6 + 5C6H12 = 6C7H16$  269 686 -269 614  
(sSfp-sSfl)=-7.18799999998882E+0001 T0s= -7484  
t0= -7484

6)  $2C2H2 + 2C7H16 = 3C6H12$  -88 301 198 214  
(sSfp-sSfl)=-8.66999999999534E+0001 T0s= 3300  
t0= 3300

7)  $1CH4 + 1C6H12 = 1C7H16$  45 116 -47 102

(sSfp-sSfl)=-1.35400000000373E+0001 T0s= -6809  
t0= -6809

8) 3C + 3C7H16 = 4C6H12 -118 311 135 285  
(sSfp-sSfl)=-2.58059999998659E+0001 T0s= 9779  
t0= 9779

9) 2C4H10 + 1C7H16 = 3C5H12 -111 251 -15 246  
(sSfp-sSfl)=-4.14999999990687E+0000 T0s= 22973  
t0= 22973

10) 2C4H6 + 11C5H12 = 9C7H16 404 1039 -336 920  
(sSfp-sSfl)=-1.18309999999590E+0002 T0s= -6256  
t0= -6256

11) 1C3H4 + 5C5H12 = 4C7H16 180 469 -139 409  
(sSfp-sSfl)=-5.98199999998324E+0001 T0s= -5319  
t0= -5319

12) 2C2H6 + 3C7H16 = 5C5H12 -185 417 94 411  
(sSfp-sSfl)=-5.91000000014901E+0000 T0s= 47164  
t0= 47164

13) 2C2H2 + 9C5H12 = 7C7H16 314 835 -224 716  
(sSfp-sSfl)=-1.19189999999478E+0002 T0s= -4517  
t0= -4517

14) 1CH4 + 2C7H16 = 3C5H12 -111 249 72 246  
(sSfp-sSfl)=-2.70999999996275E+0000 T0s= 67395  
t0= 67395

15) 1C + 4C5H12 = 3C7H16 135 330 -148 307  
(sSfp-sSfl)=-2.30419999998994E+0001 T0s= -12252  
t0= -12252

16) 3C4H6 + 11C4H10 = 8C7H16 359 1018 -227 818  
(sSfp-sSfl)=-2.0029000000037E+0002 T0s= -2925  
t0= -2925

17) 3C3H4 + 10C4H10 = 7C7H16 314 916 -164 716

(sSfp-sSfl)=-2.00209999999031E+0002 T0s= -2387

t0= -2387

18) 3C2H6 + 2C7H16 = 5C4H10 -151 369 29 371

(sSfp-sSfl)= 1.50999999977648E+0000 T0s=-119046

t0=-119046

19) 1C2H2 + 3C4H10 = 2C7H16 90 270 -36 205

(sSfp-sSfl)=-6.58199999998324E+0001 T0s= -1917

t0= -1917

20) 1CH4 + 1C7H16 = 2C4H10 -60 147 27 148

(sSfp-sSfl)= 1.43999999994412E+0000 T0s= -60625

t0= -60625

21) 3C + 8C4H10 = 5C7H16 224 597 -241 511

(sSfp-sSfl)=-8.57260000002570E+0001 T0s= -5431

t0= -5431

22) 11C3H4 + 1C7H16 = 10C4H6 350 744 550 677

(sSfp-sSfl)=-6.64700000006706E+0001 T0s= 3013

t0= 3013

23) 11C2H6 + 5C4H6 = 6C7H16 269 942 -48 614

(sSfp-sSfl)=-3.28279999999329E+0002 T0s= -966

t0= -966

24) 11C2H2 + 2C7H16 = 9C4H6 315 733 684 609

(sSfp-sSfl)=-1.23150000000373E+0002 T0s= 2998

t0= 2998

25) 11CH4 + 6C4H6 = 5C7H16 224 896 13 511

(sSfp-sSfl)=-3.84740000000689E+0002 T0s= -549

t0= -549

26) 11C + 3C7H16 = 8C4H6 280 322 135 542

(sSfp-sSfl)= 2.19777999999467E+0002 T0s= 660

t0= 660

27) 2C2H6 + 1C3H4 = 1C7H16 45 168 5 102

(sSfp-sSfl)=-6.5729999999814E+0001 T0s= -600

t0= -600

28) 10C2H2 + 1C7H16 = 9C3H4 413 582 585 525

(sSfp-sSfl)=-5.75700000002980E+0001 T0s= 2984

t0= 2984

29) 5CH4 + 3C3H4 = 2C7H16 90 398 48 205

(sSfp-sSfl)=-1.93010000000242E+0002 T0s= -214

t0= -214

30) 5C + 1C7H16 = 4C3H4 184 109 45 233

(sSfp-sSfl)= 1.24069999999949E+0002 T0s= 1119

t0= 1119

31) 5C2H2 + 9C2H6 = 4C7H16 180 734 88 409

(sSfp-sSfl)=-3.24569999999367E+0002 T0s= -282

t0= -282

32) 5CH4 + 1C7H16 = 6C2H6 -122 325 -45 329

(sSfp-sSfl)= 4.17999999970198E+0000 T0s= -18416

t0= -18416

33) 5C + 8C2H6 = 3C7H16 135 446 -162 307

(sSfp-sSfl)=-1.38849999999627E+0002 T0s= -2136

t0= -2136

34) 3CH4 + 2C2H2 = 1C7H16 45 230 54 102

(sSfp-sSfl)=-1.27320000000065E+0002 T0s= 75

t0= 75

35) 9C + 1C7H16 = 8C2H2 432 115 45 384

(sSfp-sSfl)= 2.69381999999983E+0002 T0s= 1438

t0= 1438

36) 3C + 4CH4 = 1C7H16 45 182 -72 102

(sSfp-sSfl)=-7.99660000000149E+0001 T0s= -1456

t0= -1456

37) 6C4H10 + 1C6H12 = 6C5H12 -222 516 -210 493

(sSfp-sSfl)=-2.32799999997951E+0001 T0s= 481

t0= 481

38) 2C4H6 + 2C5H12 = 3C6H12 -88 300 -4 214

(sSfp-sSfl)=-8.58200000000652E+0001 T0s= 983

t0= 983

39) 3C3H4 + 3C5H12 = 4C6H12 -118 421 27 285

(sSfp-sSfl)=-1.36139999999665E+0002 T0s= 1063

t0= 1063

40) 2C2H6 + 1C6H12 = 2C5H12 -74 181 -70 164

(sSfp-sSfl)=-1.67399999999907E+0001 T0s= 234

t0= 234

41) 6C2H2 + 6C5H12 = 7C6H12 -206 781 103 499

(sSfp-sSfl)=-2.81759999999311E+0002 T0s= 1095

t0= 1095

42) 3CH4 + 2C6H12 = 3C5H12 -111 276 -113 246

(sSfp-sSfl)=-2.97900000002701E+0001 T0s= -58

t0= -58

43) 1C + 1C5H12 = 1C6H12 -29 83 -37 71

(sSfp-sSfl)=-1.22119999999413E+0001 T0s= -613

t0= -613

44) 3C4H6 + 3C4H10 = 4C6H12 -118 425 14 285

(sSfp-sSfl)=-1.40369999999646E+0002 T0s= 942

t0= 942

45) 6C3H4 + 6C4H10 = 7C6H12 -206 795 95 499

(sSfp-sSfl)=-2.95559999999125E+0002 T0s= 1017

t0= 1017

46) 3C2H6 + 1C6H12 = 3C4H10 -90 236 -90 222

(sSfp-sSfl)=-1.34699999999721E+0001 T0s= 20

t0= 20

47) 1C2H2 + 1C4H10 = 1C6H12 -29 122 24 71

(sSfp-sSfl)=-5.08399999999674E+0001 T0s= 1048

t0= 1048

48) 2CH<sub>4</sub> + 1C<sub>6</sub>H<sub>12</sub> = 2C<sub>4</sub>H<sub>10</sub> -60 160 -65 148

(sSfp-sSfl)=-1.21000000000931E+0001 T0s= -404

t0= -404

49) 6C + 6C<sub>4</sub>H<sub>10</sub> = 5C<sub>6</sub>H<sub>12</sub> -147 453 -181 356

(sSfp-sSfl)=-9.65519999996759E+0001 T0s= -350

t0= -350

50) 6C<sub>3</sub>H<sub>4</sub> + 1C<sub>6</sub>H<sub>12</sub> = 6C<sub>4</sub>H<sub>6</sub> 210 421 246 406

(sSfp-sSfl)=-1.48200000002980E+0001 T0s= 2447

t0= 2447

51) 1C<sub>2</sub>H<sub>6</sub> + 1C<sub>4</sub>H<sub>6</sub> = 1C<sub>6</sub>H<sub>12</sub> -29 123 15 71

(sSfp-sSfl)=-5.12799999999115E+0001 T0s= 861

t0= 861

52) 3C<sub>2</sub>H<sub>2</sub> + 1C<sub>6</sub>H<sub>12</sub> = 3C<sub>4</sub>H<sub>6</sub> 105 215 133 203

(sSfp-sSfl)=-1.21500000001397E+0001 T0s= 2281

t0= 2281

53) 6CH<sub>4</sub> + 6C<sub>4</sub>H<sub>6</sub> = 5C<sub>6</sub>H<sub>12</sub> -147 673 103 356

(sSfp-sSfl)=-3.17040000000037E+0002 T0s= 788

t0= 788

54) 2C + 1C<sub>6</sub>H<sub>12</sub> = 2C<sub>4</sub>H<sub>6</sub> 70 74 -29 135

(sSfp-sSfl)= 6.13959999999497E+0001 T0s= 1619

t0= 1619

55) 6C<sub>2</sub>H<sub>6</sub> + 6C<sub>3</sub>H<sub>4</sub> = 5C<sub>6</sub>H<sub>12</sub> -147 679 154 356

(sSfp-sSfl)=-3.22500000000000E+0002 T0s= 934

t0= 934

56) 6C<sub>2</sub>H<sub>2</sub> + 1C<sub>6</sub>H<sub>12</sub> = 6C<sub>3</sub>H<sub>4</sub> 276 359 295 350

(sSfp-sSfl)=-9.48000000044703E+0000 T0s= 2022

t0= 2022

57) 3CH<sub>4</sub> + 3C<sub>3</sub>H<sub>4</sub> = 2C<sub>6</sub>H<sub>12</sub> -59 308 84 143



(sSfp-sSfl)=-1.65930000000168E+0002 T0s= 862

t0= 862

58)  $3C + 1C6H12 = 3C3H4$  138 75 -29 175

(sSfp-sSfl)= 9.95039999998407E+0001 T0s= 1680

t0= 1680

59)  $3C2H2 + 3C2H6 = 2C6H12$  -59 309 101 143

(sSfp-sSfl)=-1.65989999999758E+0002 T0s= 965

t0= 965

60)  $6CH4 + 1C6H12 = 6C2H6$  -122 338 -137 329

(sSfp-sSfl)=-9.36000000033528E+0000 T0s= -1625

t0= -1625

61)  $2C + 2C2H6 = 1C6H12$  -29 112 -41 71

(sSfp-sSfl)=-4.11639999998733E+0001 T0s= -269

t0= -269

62)  $2CH4 + 2C2H2 = 1C6H12$  -29 185 72 71

(sSfp-sSfl)=-1.13780000000028E+0002 T0s= 894

t0= 894

63)  $6C + 1C6H12 = 6C2H2$  324 80 -29 288

(sSfp-sSfl)= 2.08488000000012E+0002 T0s= 1696

t0= 1696

64)  $3C + 3CH4 = 1C6H12$  -29 138 -54 71

(sSfp-sSfl)=-6.64259999999776E+0001 T0s= -364

t0= -364

65)  $1C4H6 + 9C4H10 = 8C5H12$  -295 735 -236 657

(sSfp-sSfl)=-7.78300000000745E+0001 T0s= 758

t0= 758

66)  $1C3H4 + 8C4H10 = 7C5H12$  -258 651 -195 575

(sSfp-sSfl)=-7.64199999999255E+0001 T0s= 826

t0= 826

67)  $1C2H6 + 2C5H12 = 3C4H10$  -90 219 -94 222

(sSfp-sSfl)= 3.27000000001863E+0000 T0s= 1113

t0= 1113

68) 1C2H2 + 7C4H10 = 6C5H12 -222 567 -157 493

(sSfp-sSfl)=-7.41199999996461E+0001 T0s= 870

t0= 870

69) 1CH4 + 3C5H12 = 4C4H10 -121 291 -129 296

(sSfp-sSfl)= 5.58999999985099E+0000 T0s= 1438

t0= 1438

70) 1C + 6C4H10 = 5C5H12 -185 446 -181 411

(sSfp-sSfl)=-3.54920000000857E+0001 T0s= 104

t0= 104

71) 9C3H4 + 1C5H12 = 8C4H6 280 607 376 542

(sSfp-sSfl)=-6.51400000005960E+0001 T0s= 1483

t0= 1483

72) 3C2H6 + 1C4H6 = 2C5H12 -74 232 -26 164

(sSfp-sSfl)=-6.80200000000186E+0001 T0s= 707

t0= 707

73) 9C2H2 + 2C5H12 = 7C4H6 245 596 412 474

(sSfp-sSfl)=-1.222700000000484E+0002 T0s= 1370

t0= 1370

74) 9CH4 + 4C4H6 = 5C5H12 -185 672 -21 411

(sSfp-sSfl)=-2.610100000000242E+0002 T0s= 627

t0= 627

75) 3C + 1C5H12 = 2C4H6 70 86 -37 135

(sSfp-sSfl)= 4.91839999998920E+0001 T0s= 2173

t0= 2173

76) 8C2H6 + 3C3H4 = 5C5H12 -185 614 -24 411

(sSfp-sSfl)=-2.03100000000093E+0002 T0s= 790

t0= 790

77) 8C2H2 + 1C5H12 = 7C3H4 321 466 395 408

(sSfp-sSfl)=-5.80200000000186E+0001 T0s= 1272

t0= 1272

78) 2CH<sub>4</sub> + 1C<sub>3</sub>H<sub>4</sub> = 1C<sub>5</sub>H<sub>12</sub> -37 147 10 82

(sSfp-sSfl)=-6.52400000001071E+0001 T0s= 722

t0= 722

79) 4C + 1C<sub>5</sub>H<sub>12</sub> = 3C<sub>3</sub>H<sub>4</sub> 138 88 -37 175

(sSfp-sSfl)= 8.72919999998994E+0001 T0s= 2001

t0= 2001

80) 3C<sub>2</sub>H<sub>2</sub> + 7C<sub>2</sub>H<sub>6</sub> = 4C<sub>5</sub>H<sub>12</sub> -148 528 20 328

(sSfp-sSfl)=-1.99470000000205E+0002 T0s= 842

t0= 842

81) 3CH<sub>4</sub> + 1C<sub>5</sub>H<sub>12</sub> = 4C<sub>2</sub>H<sub>6</sub> -81 216 -91 219

(sSfp-sSfl)= 3.68999999971129E+0000 T0s= 2591

t0= 2591

82) 1C + 2C<sub>2</sub>H<sub>6</sub> = 1C<sub>5</sub>H<sub>12</sub> -37 111 -41 82

(sSfp-sSfl)=-2.89519999999320E+0001 T0s= -124

t0= -124

83) 7CH<sub>4</sub> + 4C<sub>2</sub>H<sub>2</sub> = 3C<sub>5</sub>H<sub>12</sub> -111 504 91 246

(sSfp-sSfl)=-2.57350000000326E+0002 T0s= 784

t0= 784

84) 7C + 1C<sub>5</sub>H<sub>12</sub> = 6C<sub>2</sub>H<sub>2</sub> 324 92 -37 288

(sSfp-sSfl)= 1.96275999999954E+0002 T0s= 1839

t0= 1839

85) 2C + 3CH<sub>4</sub> = 1C<sub>5</sub>H<sub>12</sub> -37 136 -54 82

(sSfp-sSfl)=-5.42140000000363E+0001 T0s= -308

t0= -308

86) 8C<sub>3</sub>H<sub>4</sub> + 1C<sub>4</sub>H<sub>10</sub> = 7C<sub>4</sub>H<sub>6</sub> 245 541 337 474

(sSfp-sSfl)=-6.65499999998137E+0001 T0s= 1389

t0= 1389

87) 4C<sub>2</sub>H<sub>6</sub> + 1C<sub>4</sub>H<sub>6</sub> = 3C<sub>4</sub>H<sub>10</sub> -90 287 -46 222

(sSfp-sSfl)=-6.47499999997672E+0001 T0s= 686

t0= 686

88) 4C2H2 + 1C4H10 = 3C4H6 105 266 186 203

(sSfp-sSfl)=-6.29900000002235E+0001 T0s= 1286

t0= 1286

89) 8CH4 + 3C4H6 = 5C4H10 -151 559 -38 371

(sSfp-sSfl)=-1.88770000000019E+0002 T0s= 597

t0= 597

90) 8C + 3C4H10 = 5C4H6 175 233 -90 339

(sSfp-sSfl)= 1.05213999999920E+0002 T0s= 2522

t0= 2522

91) 7C2H6 + 2C3H4 = 5C4H10 -151 501 -50 371

(sSfp-sSfl)=-1.29949999999721E+0002 T0s= 776

t0= 776

92) 7C2H2 + 1C4H10 = 6C3H4 276 410 348 350

(sSfp-sSfl)=-6.03200000002980E+0001 T0s= 1201

t0= 1201

93) 7CH4 + 3C3H4 = 4C4H10 -121 487 13 296

(sSfp-sSfl)=-1.901300000000354E+0002 T0s= 701

t0= 701

94) 7C + 2C4H10 = 5C3H4 230 158 -60 292

(sSfp-sSfl)= 1.33655999999959E+0002 T0s= 2169

t0= 2169

95) 1C2H2 + 3C2H6 = 2C4H10 -60 213 -7 148

(sSfp-sSfl)=-6.43100000000559E+0001 T0s= 833

t0= 833

96) 2CH4 + 1C4H10 = 3C2H6 -61 163 -66 165

(sSfp-sSfl)= 1.36999999987893E+0000 T0s= 3766

t0= 3766

97) 2C + 5C2H6 = 3C4H10 -90 277 -101 222

(sSfp-sSfl)=-5.46339999998454E+0001 T0s= -198

t0= -198

98) 2CH<sub>4</sub> + 1C<sub>2</sub>H<sub>2</sub> = 1C<sub>4</sub>H<sub>10</sub> -30 137 18 74

(sSfp-sSfl)=-6.29400000000605E+0001 T0s= 769

t0= 769

99) 6C + 1C<sub>4</sub>H<sub>10</sub> = 5C<sub>2</sub>H<sub>2</sub> 270 82 -30 240

(sSfp-sSfl)= 1.57648000000045E+0002 T0s= 1905

t0= 1905

100) 3C + 5CH<sub>4</sub> = 2C<sub>4</sub>H<sub>10</sub> -60 227 -89 148

(sSfp-sSfl)=-7.85260000000708E+0001 T0s= -371

t0= -371

101) 1C<sub>2</sub>H<sub>6</sub> + 6C<sub>3</sub>H<sub>4</sub> = 5C<sub>4</sub>H<sub>6</sub> 175 405 255 339

(sSfp-sSfl)=-6.61000000000931E+0001 T0s= 1217

t0= 1217

102) 1C<sub>2</sub>H<sub>2</sub> + 1C<sub>4</sub>H<sub>6</sub> = 2C<sub>3</sub>H<sub>4</sub> 92 116 89 117

(sSfp-sSfl)= 8.90000000013970E-0001 T0s= 3202

t0= 3202

103) 1CH<sub>4</sub> + 5C<sub>3</sub>H<sub>4</sub> = 4C<sub>4</sub>H<sub>6</sub> 140 336 212 271

(sSfp-sSfl)=-6.51899999999441E+0001 T0s= 1102

t0= 1102

104) 1C + 2C<sub>4</sub>H<sub>6</sub> = 3C<sub>3</sub>H<sub>4</sub> 138 137 70 175

(sSfp-sSfl)= 3.81080000000075E+0001 T0s= 1780

t0= 1780

105) 3C<sub>2</sub>H<sub>2</sub> + 1C<sub>2</sub>H<sub>6</sub> = 2C<sub>4</sub>H<sub>6</sub> 70 199 142 135

(sSfp-sSfl)=-6.34300000001676E+0001 T0s= 1133

t0= 1133

106) 6CH<sub>4</sub> + 1C<sub>4</sub>H<sub>6</sub> = 5C<sub>2</sub>H<sub>6</sub> -101 335 -72 274

(sSfp-sSfl)=-6.06400000001304E+0001 T0s= 477

t0= 477

107) 2C + 1C<sub>2</sub>H<sub>6</sub> = 1C<sub>4</sub>H<sub>6</sub> 35 58 -20 68

(sSfp-sSfl)= 1.0115999999800E+0001 T0s= 5459

t0= 5459

108) 2CH<sub>4</sub> + 5C<sub>2</sub>H<sub>2</sub> = 3C<sub>4</sub>H<sub>6</sub> 105 329 234 203

(sSfp-sSfl)=-1.25930000000168E+0002 T0s= 1028

t0= 1028

109) 2C + 1C<sub>4</sub>H<sub>6</sub> = 3C<sub>2</sub>H<sub>2</sub> 162 70 35 144

(sSfp-sSfl)= 7.35460000000894E+0001 T0s= 1728

t0= 1728

110) 5C + 3CH<sub>4</sub> = 2C<sub>4</sub>H<sub>6</sub> 70 140 -54 135

(sSfp-sSfl)=-5.03000000026077E+0000 T0s= -24569

t0= -24569

111) 5C<sub>2</sub>H<sub>2</sub> + 1C<sub>2</sub>H<sub>6</sub> = 4C<sub>3</sub>H<sub>4</sub> 184 295 250 233

(sSfp-sSfl)=-6.16500000001397E+0001 T0s= 1073

t0= 1073

112) 5CH<sub>4</sub> + 1C<sub>3</sub>H<sub>4</sub> = 4C<sub>2</sub>H<sub>6</sub> -81 281 -43 219

(sSfp-sSfl)=-6.15500000002794E+0001 T0s= 610

t0= 610

113) 5C + 2C<sub>2</sub>H<sub>6</sub> = 3C<sub>3</sub>H<sub>4</sub> 138 117 -41 175

(sSfp-sSfl)= 5.8339999999674E+0001 T0s= 3056

t0= 3056

114) 1CH<sub>4</sub> + 4C<sub>2</sub>H<sub>2</sub> = 3C<sub>3</sub>H<sub>4</sub> 138 237 198 175

(sSfp-sSfl)=-6.16300000001211E+0001 T0s= 981

t0= 981

115) 1C + 1C<sub>3</sub>H<sub>4</sub> = 2C<sub>2</sub>H<sub>2</sub> 108 60 46 96

(sSfp-sSfl)= 3.63280000000377E+0001 T0s= 1710

t0= 1710

116) 2C + 1CH<sub>4</sub> = 1C<sub>3</sub>H<sub>4</sub> 46 47 -18 58

(sSfp-sSfl)= 1.10259999999544E+0001 T0s= 5786

t0= 5786

117) 4CH<sub>4</sub> + 1C<sub>2</sub>H<sub>2</sub> = 3C<sub>2</sub>H<sub>6</sub> -61 226 -18 165

(sSfp-sSfl)=-6.15700000000652E+0001 T0s= 702

t0= 702

118)  $4C + 1C_2H_6 = 3C_2H_2$  162 60 -20 144

(sSfp-sSfl)= 8.36620000000112E+0001 T0s= 2179

t0= 2179

119)  $1C + 3CH_4 = 2C_2H_6$  -41 135 -54 110

(sSfp-sSfl)=-2.52620000001043E+0001 T0s= -520

t0= -520

120)  $3C + 1CH_4 = 2C_2H_2$  108 49 -18 96

(sSfp-sSfl)= 4.73539999999921E+0001 T0s= 2659

t0= 2659

121)  $3O_2 + 6C_7H_{16} = 7C_6H_{12} + 6H_2O$  -553 761 269 770

(sSfp-sSfl)= 8.96100000012666E+0000 T0s= -91738

t0= -91738

122)  $1O_2 + 7C_5H_{12} = 5C_7H_{16} + 2H_2O$  109 624 -258 602

(sSfp-sSfl)=-2.22829999998212E+0001 T0s= -16481

t0= -16481

123)  $3O_2 + 14C_4H_{10} = 8C_7H_{16} + 6H_2O$  12 1185 -422 1089

(sSfp-sSfl)=-9.58990000002086E+0001 T0s= -4529

t0= -4529

124)  $11O_2 + 8C_7H_{16} = 14C_4H_6 + 22H_2O$  -782 1357 359 1940

(sSfp-sSfl)= 5.83057000000030E+0002 T0s= -1957

t0= -1957

125)  $5O_2 + 3C_7H_{16} = 7C_3H_4 + 10H_2O$  -257 552 135 859

(sSfp-sSfl)= 3.07325000000186E+0002 T0s= -1273

t0= -1273

126)  $5O_2 + 14C_2H_6 = 4C_7H_{16} + 10H_2O$  -398 1013 -284 860

(sSfp-sSfl)=-1.52784999999218E+0002 T0s= 752

t0= 752

127)  $9O_2 + 4C_7H_{16} = 14C_2H_2 + 18H_2O$  -284 850 180 1484

(sSfp-sSfl)= 6.33782999999821E+0002 T0s= -731

t0= -731

128) 3O<sub>2</sub> + 7CH<sub>4</sub> = 1C<sub>7</sub>H<sub>16</sub> + 6H<sub>2</sub>O -302 459 -125 373

(sSfp-sSfl)=-8.58190000001341E+0001 T0s= 2059

t0= 2059

129) 7C + 8H<sub>2</sub>O = 4O<sub>2</sub> + 1C<sub>7</sub>H<sub>16</sub> 45 370 -462 298

(sSfp-sSfl)=-7.21620000000112E+0001 T0s= -7029

t0= -7029

130) 3O<sub>2</sub> + 6C<sub>5</sub>H<sub>12</sub> = 5C<sub>6</sub>H<sub>12</sub> + 6H<sub>2</sub>O -494 640 -222 627

(sSfp-sSfl)=-1.26990000000224E+0001 T0s= 21451

t0= 21451

131) 3O<sub>2</sub> + 6C<sub>4</sub>H<sub>10</sub> = 4C<sub>6</sub>H<sub>12</sub> + 6H<sub>2</sub>O -464 592 -181 556

(sSfp-sSfl)=-3.59790000002831E+0001 T0s= 7882

t0= 7882

132) 3O<sub>2</sub> + 4C<sub>6</sub>H<sub>12</sub> = 6C<sub>4</sub>H<sub>6</sub> + 6H<sub>2</sub>O -137 432 -118 677

(sSfp-sSfl)= 2.44760999999475E+0002 T0s= -79

t0= -79

133) 1O<sub>2</sub> + 1C<sub>6</sub>H<sub>12</sub> = 2C<sub>3</sub>H<sub>4</sub> + 2H<sub>2</sub>O -24 120 -29 207

(sSfp-sSfl)= 8.65270000001183E+0001 T0s= 66

t0= 66

134) 3O<sub>2</sub> + 6C<sub>2</sub>H<sub>6</sub> = 2C<sub>6</sub>H<sub>12</sub> + 6H<sub>2</sub>O -406 476 -122 413

(sSfp-sSfl)=-6.29189999997616E+0001 T0s= 4516

t0= 4516

135) 3O<sub>2</sub> + 2C<sub>6</sub>H<sub>12</sub> = 6C<sub>2</sub>H<sub>2</sub> + 6H<sub>2</sub>O -23 290 -59 559

(sSfp-sSfl)= 2.69060999999754E+0002 T0s= 135

t0= 135

136) 3O<sub>2</sub> + 6CH<sub>4</sub> = 1C<sub>6</sub>H<sub>12</sub> + 6H<sub>2</sub>O -376 414 -107 342

(sSfp-sSfl)=-7.22790000000969E+0001 T0s= 3721

t0= 3721

137) 6C + 6H<sub>2</sub>O = 3O<sub>2</sub> + 1C<sub>6</sub>H<sub>12</sub> -29 279 -347 218



(sSfp-sSfl)=-6.05730000000913E+0001 T0s= -5239

t0= -5239

138) 1O2 + 10C4H10 = 8C5H12 + 2H2O -411 790 -302 747

(sSfp-sSfl)=-4.30329999998212E+0001 T0s= 2543

t0= 2543

139) 9O2 + 8C5H12 = 10C4H6 + 18H2O -691 1098 -295 1489

(sSfp-sSfl)= 3.91002999998629E+0002 T0s= -1011

t0= -1011

140) 4O2 + 3C5H12 = 5C3H4 + 8H2O -233 442 -111 652

(sSfp-sSfl)= 2.09968000000343E+0002 T0s= -581

t0= -581

141) 3O2 + 10C2H6 = 4C5H12 + 6H2O -494 696 -203 599

(sSfp-sSfl)=-9.63989999992773E+0001 T0s= 3029

t0= 3029

142) 7O2 + 4C5H12 = 10C2H2 + 14H2O -269 672 -148 1111

(sSfp-sSfl)= 4.39969000000507E+0002 T0s= -276

t0= -276

143) 2O2 + 5CH4 = 1C5H12 + 4H2O -268 321 -89 263

(sSfp-sSfl)=-5.81159999999218E+0001 T0s= 3075

t0= 3075

144) 5C + 6H2O = 3O2 + 1C5H12 -37 277 -347 229

(sSfp-sSfl)=-4.83610000000335E+0001 T0s= -6407

t0= -6407

145) 1O2 + 1C4H10 = 1C4H6 + 2H2O -81 123 -30 158

(sSfp-sSfl)= 3.47970000000205E+0001 T0s= -1450

t0= -1450

146) 7O2 + 6C4H10 = 8C3H4 + 14H2O -442 788 -181 1098

(sSfp-sSfl)= 3.10128999999724E+0002 T0s= -841

t0= -841

147) 1O2 + 4C2H6 = 2C4H10 + 2H2O -176 268 -81 238

(sSfp-sSfl)=-2.99529999997467E+0001 T0s= 3168

t0= 3168

148)  $3O_2 + 2C_4H_{10} = 4C_2H_2 + 6H_2O$  -131 295 -60 463

(sSfp-sSfl)= 1.67381000000052E+0002 T0s= -421

t0= -421

149)  $3O_2 + 8CH_4 = 2C_4H_{10} + 6H_2O$  -407 503 -143 419

(sSfp-sSfl)=-8.43790000001900E+0001 T0s= 3129

t0= 3129

150)  $8C + 10H_2O = 5O_2 + 2C_4H_{10}$  -60 462 -578 393

(sSfp-sSfl)=-6.87710000001825E+0001 T0s= -7527

t0= -7527

151)  $1O_2 + 6C_4H_6 = 8C_3H_4 + 2H_2O$  252 455 210 557

(sSfp-sSfl)= 1.01347000000067E+0002 T0s= 414

t0= 414

152)  $3O_2 + 4C_2H_6 = 2C_4H_6 + 6H_2O$  -277 366 -81 406

(sSfp-sSfl)= 3.96410000002943E+0001 T0s= -4940

t0= -4940

153)  $1O_2 + 2C_4H_6 = 4C_2H_2 + 2H_2O$  100 184 70 282

(sSfp-sSfl)= 9.77870000002440E+0001 T0s= 312

t0= 312

154)  $5O_2 + 8CH_4 = 2C_4H_6 + 10H_2O$  -508 601 -143 586

(sSfp-sSfl)=-1.47850000001490E+0001 T0s= 24686

t0= 24686

155)  $8C + 6H_2O = 3O_2 + 2C_4H_6$  70 282 -347 282

(sSfp-sSfl)= 8.22999999858439E-0001 T0s= 506338

t0= 506338

156)  $5O_2 + 6C_2H_6 = 4C_3H_4 + 10H_2O$  -394 574 -122 684

(sSfp-sSfl)= 1.10135000000708E+0002 T0s= -2477

t0= -2477

157)  $1O_2 + 4C_3H_4 = 6C_2H_2 + 2H_2O$  209 282 184 378

(sSfp-sSfl)= 9.60070000002161E+0001 T0s= 259

t0= 259

158)  $2O_2 + 3CH_4 = 1C_3H_4 + 4H_2O$  -185 232 -54 239

(sSfp-sSfl)= 7.12400000006892E+0000 T0s= -18476

t0= -18476

159)  $3C + 2H_2O = 1O_2 + 1C_3H_4$  46 94 -116 107

(sSfp-sSfl)= 1.29769999999553E+0001 T0s= 12446

t0= 12446

160)  $1O_2 + 1C_2H_6 = 1C_2H_2 + 2H_2O$  -62 104 -20 138

(sSfp-sSfl)= 3.43570000000764E+0001 T0s= -1203

t0= -1203

161)  $1O_2 + 4CH_4 = 2C_2H_6 + 2H_2O$  -156 227 -72 200

(sSfp-sSfl)=-2.72130000002217E+0001 T0s= 3108

t0= 3108

162)  $4C + 6H_2O = 3O_2 + 2C_2H_6$  -41 276 -347 257

(sSfp-sSfl)=-1.94089999999851E+0001 T0s= -15780

t0= -15780

163)  $3O_2 + 4CH_4 = 2C_2H_2 + 6H_2O$  -239 325 -72 367

(sSfp-sSfl)= 4.15010000001639E+0001 T0s= -4029

t0= -4029

164)  $4C + 2H_2O = 1O_2 + 2C_2H_2$  108 96 -116 145

(sSfp-sSfl)= 4.93050000000512E+0001 T0s= 4536

t0= 4536

165)  $1C + 2H_2O = 1O_2 + 1CH_4$  -18 92 -116 94

(sSfp-sSfl)= 1.95100000000093E+0000 T0s= 50083

t0= 50083

Список завершен

Сортировка и выбор группы базовых реакций

258 288 300 274 324 328 318 310 330 72

253 249 240 247 66 232 325 236 315 319

307 241 50 220 68 58 311 295 42 198  
 283 303 128 46 14 168 54 62 271 30  
 10 226 291 170 32 4 34 279 38 20  
 2 289 22 26 126 200 277 269 285 214  
 27 297 267 11 188 39 23 158 244 7  
 265 218 15 238 35 122 5 263 321 180  
 246 70 116 261 150 47 230 281 259 305  
 164 63 255 293 17 194 313 108 55 98

Порядковые номера реакций в группе с max потенциалом:

258 288 300 274 324 328 318 310 330  
 -129 -144 -150 -137 -162 -164 -159 -155 -165

Термодинамический потенциал суммарный в указанных ед. (кал/г)

dgs= -2161.383

Примечание. Знак (-) перед реакцией означает противоположное направление реакции. Отрицательная температура условно допускается. Знак (sSfp-sSfl) означает направление прямой энергии Гиббса. T0 – это температура при которой энергия Гиббса равна нулю.

- 129)  $7C + 8H_2O = 4O_2 + 1C_7H_{16}$  45 370 -462 298
- 144)  $5C + 6H_2O = 3O_2 + 1C_5H_{12}$  -37 277 -347 229
- 150)  $8C + 10H_2O = 5O_2 + 2C_4H_{10}$  -60 462 -578 393
- 137)  $6C + 6H_2O = 3O_2 + 1C_6H_{12}$  -29 279 -347 218
- 162)  $4C + 6H_2O = 3O_2 + 2C_2H_6$  -41 276 -347 257
- 164)  $4C + 2H_2O = 1O_2 + 2C_2H_2$  108 96 -116 145
- 159)  $3C + 2H_2O = 1O_2 + 1C_3H_4$  46 94 -116 107
- 155)  $8C + 6H_2O = 3O_2 + 2C_4H_6$  70 282 -347 282
- 165)  $1C + 2H_2O = 1O_2 + 1CH_4$  -18 92 -116 94

В итоге мы видим при температуре 1000 К расклад линейно независимых реакций с образованием углерода и паров воды. Если мы хотим получить углеводороды из углерода надо исключить кислород из начальных данных.

Группа элементов C-H

Начальные данные

nb= 2 np= 12 tk=1000 K

Атомные веса элементов:

12.00 1.01

Наименования веществ dhf,ккал/мол s0,ккал/град.мол

C	0.000	1.372
CH4	-17.880	44.530
C2H2	54.020	48.000
C2H6	-20.250	54.850
C3H4	45.920	58.300
C3H6	12.740	56.750
C4H6	34.970	67.710
C4H10	-30.150	74.120
C5H12	-36.920	82.120
C6H12	-29.430	71.280
C7H16	44.880	102.270
C10H8	18.660	39.890

Матрица групп элементов в веществах

1.0 0.0  
1.0 4.0  
2.0 2.0  
2.0 6.0  
3.0 4.0  
3.0 6.0  
4.0 6.0  
4.0 10.0  
5.0 12.0  
6.0 12.0  
7.0 16.0  
10.0 8.0

## Расчетные данные

- 1)  $26C6H_{12} = 18C7H_{16} + 3C_{10}H_8$  864 1853 -765 1961  
(sSfp-sSfl)= 1.072500000000000E+0002 T0s= 15189  
t0= 15189
- 2)  $26C5H_{12} + 1C_{10}H_8 = 20C7H_{16}$  898 2175 -941 2045  
(sSfp-sSfl)=-1.29610000001267E+0002 T0s= -14188  
t0= -14188
- 3)  $52C4H_{10} + 3C_{10}H_8 = 34C7H_{16}$  1526 3974 -1512 3477  
(sSfp-sSfl)=-4.96730000000447E+0002 T0s= -6115  
t0= -6115
- 4)  $52C4H_6 = 14C7H_{16} + 11C_{10}H_8$  834 3521 1818 1871  
(sSfp-sSfl)=-1.65034999999590E+0003 T0s= 597  
t0= 597
- 5)  $52C3H_6 = 18C7H_{16} + 3C_{10}H_8$  864 2951 662 1961  
(sSfp-sSfl)=-9.90469999998808E+0002 T0s= -203  
t0= -203
- 6)  $26C3H_4 = 4C7H_{16} + 5C_{10}H_8$  273 1516 1194 609  
(sSfp-sSfl)=-9.07269999998622E+0002 T0s= 1015  
t0= 1015
- 7)  $52C2H_6 + 5C_{10}H_8 = 22C7H_{16}$  987 3052 -960 2250  
(sSfp-sSfl)=-8.01709999997169E+0002 T0s= -2429  
t0= -2429
- 8)  $52C2H_2 = 2C7H_{16} + 9C_{10}H_8$  258 2496 2809 564  
(sSfp-sSfl)=-1.93245000000019E+0003 T0s= 1320  
t0= 1320
- 9)  $26CH_4 + 3C_{10}H_8 = 8C7H_{16}$  359 1277 -409 818  
(sSfp-sSfl)=-4.59290000000969E+0002 T0s= -1672  
t0= -1672
- 10)  $13C + 1C7H_{16} = 2C_{10}H_8$  37 120 45 80  
(sSfp-sSfl)=-4.03260000000009E+0001 T0s= 187

t0= 187

11)  $18C5H12 + 3C10H8 = 20C6H12$  -589 1598 -609 1426  
(sSfp-sSfl)=-1.72229999998584E+0002 T0s= -116

t0= -116

12)  $18C4H10 + 3C10H8 = 17C6H12$  -500 1454 -487 1212  
(sSfp-sSfl)=-2.42070000000298E+0002 T0s= 56

t0= 56

13)  $18C4H6 = 7C6H12 + 3C10H8$  -150 1219 629 619  
(sSfp-sSfl)=-6.00149999998510E+0002 T0s= 1299

t0= 1299

14)  $18C3H4 = 4C6H12 + 3C10H8$  -62 1049 827 405  
(sSfp-sSfl)=-6.44610000000335E+0002 T0s= 1378

t0= 1378

15)  $18C2H6 + 3C10H8 = 11C6H12$  -324 1107 -309 784  
(sSfp-sSfl)=-3.22890000000596E+0002 T0s= 47

t0= 47

16)  $18C2H2 = 1C6H12 + 3C10H8$  27 864 972 191  
(sSfp-sSfl)=-6.73049999999814E+0002 T0s= 1405

t0= 1405

17)  $18CH4 + 3C10H8 = 8C6H12$  -235 921 -266 570  
(sSfp-sSfl)=-3.50970000000671E+0002 T0s= -87

t0= -87

18)  $18C + 2C6H12 = 3C10H8$  56 167 -59 120  
(sSfp-sSfl)=-4.75860000000102E+0001 T0s= -2413

t0= -2413

19)  $40C4H10 + 1C10H8 = 34C5H12$  -1255 3005 -1187 2792  
(sSfp-sSfl)=-2.126100000003129E+0002 T0s= 320

t0= 320

20)  $40C4H6 = 14C5H12 + 9C10H8$  -349 2708 1399 1509  
(sSfp-sSfl)=-1.19970999999903E+0003 T0s= 1457

t0= 1457

$$21) 40C3H6 = 18C5H12 + 3C10H8 \quad -609 \quad 2270 \quad 510 \quad 1598$$

(sSfp-sSfl)=-6.72169999999925E+0002 T0s= 1664

t0= 1664

$$22) 5C3H4 = 1C5H12 + 1C10H8 \quad -18 \quad 292 \quad 230 \quad 122$$

(sSfp-sSfl)=-1.69489999999991E+0002 T0s= 1462

t0= 1462

$$23) 40C2H6 + 3C10H8 = 22C5H12 \quad -812 \quad 2314 \quad -754 \quad 1807$$

(sSfp-sSfl)=-5.07030000001192E+0002 T0s= 115

t0= 115

$$24) 40C2H2 = 2C5H12 + 7C10H8 \quad 57 \quad 1920 \quad 2161 \quad 443$$

(sSfp-sSfl)=-1.47652999999980E+0003 T0s= 1425

t0= 1425

$$25) 10CH4 + 1C10H8 = 4C5H12 \quad -148 \quad 485 \quad -160 \quad 328$$

(sSfp-sSfl)=-1.56710000000428E+0002 T0s= -80

t0= -80

$$26) 20C + 2C5H12 = 3C10H8 \quad 56 \quad 192 \quad -74 \quad 120$$

(sSfp-sSfl)=-7.20099999998929E+0001 T0s= -1803

t0= -1803

$$27) 17C4H6 = 7C4H10 + 4C10H8 \quad -136 \quad 1151 \quad 594 \quad 678$$

(sSfp-sSfl)=-4.72669999999925E+0002 T0s= 1546

t0= 1546

$$28) 34C3H6 = 18C4H10 + 3C10H8 \quad -487 \quad 1930 \quad 433 \quad 1454$$

(sSfp-sSfl)=-4.75669999999925E+0002 T0s= 1934

t0= 1934

$$29) 34C3H4 = 8C4H10 + 7C10H8 \quad -111 \quad 1982 \quad 1561 \quad 872$$

(sSfp-sSfl)=-1.11000999999885E+0003 T0s= 1506

t0= 1506

$$30) 17C2H6 + 1C10H8 = 11C4H10 \quad -332 \quad 972 \quad -326 \quad 815$$

(sSfp-sSfl)=-1.57019999998622E+0002 T0s= 39



t0= 39



(sSfp-sSfl)=-6.22209999999963E+0002 T0s= 1434

t0= 1434



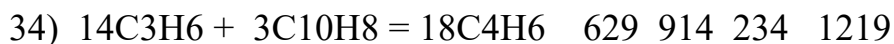
(sSfp-sSfl)=-4.47770000001416E+0002 T0s= -155

t0= -155



(sSfp-sSfl)=-1.43677999999840E+0002 T0s= -1489

t0= -1489



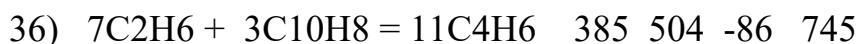
(sSfp-sSfl)= 3.04609999999404E+0002 T0s= 1297

t0= 1297



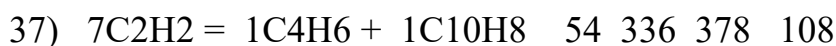
(sSfp-sSfl)=-2.34630000000820E+0002 T0s= 1468

t0= 1468



(sSfp-sSfl)= 2.41189999999944E+0002 T0s= 1950

t0= 1950



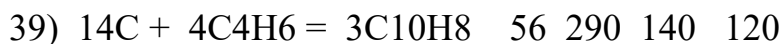
(sSfp-sSfl)=-2.28400000000023E+0002 T0s= 1421

t0= 1421



(sSfp-sSfl)= 2.60489999998361E+0002 T0s= 2751

t0= 2751



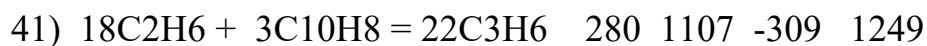
(sSfp-sSfl)=-1.70377999999910E+0002 T0s= 492

t0= 492



(sSfp-sSfl)=-4.75730000000447E+0002 T0s= 1406

t0= 1406



(sSfp-sSfl)= 1.41529999999329E+0002 T0s= 4160

t0= 4160



(sSfp-sSfl)=-6.30829999999842E+0002 T0s= 1412

t0= 1412



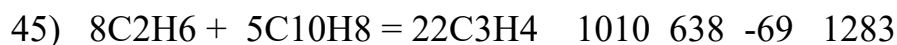
(sSfp-sSfl)=-1.32100000008941E+0001 T0s= -35556

t0= -35556



(sSfp-sSfl)=-1.32025999999954E+0002 T0s= -38

t0= -38



(sSfp-sSfl)= 6.44349999999627E+0002 T0s= 1674

t0= 1674



(sSfp-sSfl)=-2.27510000000009E+0002 T0s= 1414

t0= 1414



(sSfp-sSfl)= 1.04249999999767E+0002 T0s= 1926

t0= 1926



(sSfp-sSfl)=-8.21979999999749E+0001 T0s= 890

t0= 890



(sSfp-sSfl)=-3.93369999999879E+0002 T0s= 1467

t0= 1467



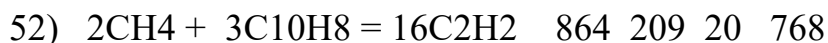
(sSfp-sSfl)=-1.41950000001118E+0002 T0s= -357

t0= -357



(sSfp-sSfl)=-1.29913999999757E+0002 T0s= -1054

t0= -1054



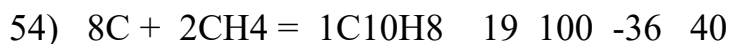
(sSfp-sSfl)= 5.59269999999786E+0002 T0s= 1509

t0= 1509



(sSfp-sSfl)=-1.54853999999934E+0002 T0s= 1275

t0= 1275



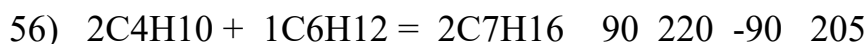
(sSfp-sSfl)=-6.01460000000661E+0001 T0s= -905

t0= -905



(sSfp-sSfl)=-1.08300000000745E+0001 T0s= -25377

t0= -25377



(sSfp-sSfl)=-1.49799999999814E+0001 T0s= -11982

t0= -11982



(sSfp-sSfl)=-2.35799999999814E+0002 T0s= 3405

t0= 3405



(sSfp-sSfl)=-1.25309999999590E+0002 T0s= 3348

t0= 3348



(sSfp-sSfl)=-7.18799999998882E+0001 T0s= -7484

t0= -7484



(sSfp-sSfl)=-8.66999999999534E+0001 T0s= 3300

t0= 3300

61) 1CH<sub>4</sub> + 1C<sub>6</sub>H<sub>12</sub> = 1C<sub>7</sub>H<sub>16</sub> 45 116 -47 102  
(sSfp-sSfl)=-1.35400000000373E+0001 T0s= -6809

t0= -6809

62) 3C + 3C<sub>7</sub>H<sub>16</sub> = 4C<sub>6</sub>H<sub>12</sub> -118 311 135 285  
(sSfp-sSfl)=-2.58059999998659E+0001 T0s= 9779

t0= 9779

63) 2C<sub>4</sub>H<sub>10</sub> + 1C<sub>7</sub>H<sub>16</sub> = 3C<sub>5</sub>H<sub>12</sub> -111 251 -15 246  
(sSfp-sSfl)=-4.14999999990687E+0000 T0s= 22973

t0= 22973

64) 2C<sub>4</sub>H<sub>6</sub> + 11C<sub>5</sub>H<sub>12</sub> = 9C<sub>7</sub>H<sub>16</sub> 404 1039 -336 920  
(sSfp-sSfl)=-1.18309999999590E+0002 T0s= -6256

t0= -6256

65) 2C<sub>3</sub>H<sub>6</sub> + 3C<sub>5</sub>H<sub>12</sub> = 3C<sub>7</sub>H<sub>16</sub> 135 360 -85 307  
(sSfp-sSfl)=-5.30499999998137E+0001 T0s= -4146

t0= -4146

66) 1C<sub>3</sub>H<sub>4</sub> + 5C<sub>5</sub>H<sub>12</sub> = 4C<sub>7</sub>H<sub>16</sub> 180 469 -139 409  
(sSfp-sSfl)=-5.98199999998324E+0001 T0s= -5319

t0= -5319

67) 2C<sub>2</sub>H<sub>6</sub> + 3C<sub>7</sub>H<sub>16</sub> = 5C<sub>5</sub>H<sub>12</sub> -185 417 94 411  
(sSfp-sSfl)=-5.91000000014901E+0000 T0s= 47164

t0= 47164

68) 2C<sub>2</sub>H<sub>2</sub> + 9C<sub>5</sub>H<sub>12</sub> = 7C<sub>7</sub>H<sub>16</sub> 314 835 -224 716  
(sSfp-sSfl)=-1.19189999999478E+0002 T0s= -4517

t0= -4517

69) 1CH<sub>4</sub> + 2C<sub>7</sub>H<sub>16</sub> = 3C<sub>5</sub>H<sub>12</sub> -111 249 72 246  
(sSfp-sSfl)=-2.70999999996275E+0000 T0s= 67395

t0= 67395

70) 1C + 4C<sub>5</sub>H<sub>12</sub> = 3C<sub>7</sub>H<sub>16</sub> 135 330 -148 307  
(sSfp-sSfl)=-2.30419999998994E+0001 T0s= -12252

t0= -12252

71) 3C4H6 + 11C4H10 = 8C7H16 359 1018 -227 818  
(sSfp-sSfl)=-2.00290000000037E+0002 T0s= -2925

t0= -2925

72) 1C3H6 + 1C4H10 = 1C7H16 45 131 -17 102  
(sSfp-sSfl)=-2.860000000000931E+0001 T0s= -2178

t0= -2178

73) 3C3H4 + 10C4H10 = 7C7H16 314 916 -164 716  
(sSfp-sSfl)=-2.00209999999031E+0002 T0s= -2387

t0= -2387

74) 3C2H6 + 2C7H16 = 5C4H10 -151 369 29 371  
(sSfp-sSfl)= 1.50999999977648E+0000 T0s=-119046

t0=-119046

75) 1C2H2 + 3C4H10 = 2C7H16 90 270 -36 205  
(sSfp-sSfl)=-6.5819999998324E+0001 T0s= -1917

t0= -1917

76) 1CH4 + 1C7H16 = 2C4H10 -60 147 27 148  
(sSfp-sSfl)= 1.4399999994412E+0000 T0s= -60625

t0= -60625

77) 3C + 8C4H10 = 5C7H16 224 597 -241 511  
(sSfp-sSfl)=-8.57260000002570E+0001 T0s= -5431

t0= -5431

78) 11C3H6 = 3C4H6 + 3C7H16 240 624 140 510  
(sSfp-sSfl)=-1.14310000000056E+0002 T0s= -870

t0= -870

79) 11C3H4 + 1C7H16 = 10C4H6 350 744 550 677  
(sSfp-sSfl)=-6.64700000006706E+0001 T0s= 3013

t0= 3013

80) 11C2H6 + 5C4H6 = 6C7H16 269 942 -48 614  
(sSfp-sSfl)=-3.28279999999329E+0002 T0s= -966

t0= -966

81) 11C2H2 + 2C7H16 = 9C4H6 315 733 684 609  
(sSfp-sSfl)=-1.23150000000373E+0002 T0s= 2998

t0= 2998

82) 11CH4 + 6C4H6 = 5C7H16 224 896 13 511  
(sSfp-sSfl)=-3.84740000000689E+0002 T0s= -549

t0= -549

83) 11C + 3C7H16 = 8C4H6 280 322 135 542  
(sSfp-sSfl)= 2.19777999999467E+0002 T0s= 660

t0= 660

84) 3C3H4 + 3C7H16 = 10C3H6 127 482 272 568  
(sSfp-sSfl)= 8.57900000000373E+0001 T0s= -1690

t0= -1690

85) 3C2H6 + 5C3H6 = 3C7H16 135 448 3 307  
(sSfp-sSfl)=-1.41490000000224E+0002 T0s= -931

t0= -931

86) 1C2H2 + 1C7H16 = 3C3H6 38 150 99 170  
(sSfp-sSfl)= 1.99799999999814E+0001 T0s= -3037

t0= -3037

87) 1CH4 + 2C3H6 = 1C7H16 45 158 8 102  
(sSfp-sSfl)=-5.57600000000093E+0001 T0s= -669

t0= -669

88) 3C + 3C7H16 = 8C3H6 102 311 135 454  
(sSfp-sSfl)= 1.43074000000022E+0002 T0s= -229

t0= -229

89) 2C2H6 + 1C3H4 = 1C7H16 45 168 5 102  
(sSfp-sSfl)=-6.57299999999814E+0001 T0s= -600

t0= -600

90) 10C2H2 + 1C7H16 = 9C3H4 413 582 585 525  
(sSfp-sSfl)=-5.75700000002980E+0001 T0s= 2984

t0= 2984

91)  $5\text{CH}_4 + 3\text{C}_3\text{H}_4 = 2\text{C}_7\text{H}_{16}$  90 398 48 205  
(sSfp-sSfl)=-1.93010000000242E+0002 T0s= -214

t0= -214

92)  $5\text{C} + 1\text{C}_7\text{H}_{16} = 4\text{C}_3\text{H}_4$  184 109 45 233  
(sSfp-sSfl)= 1.24069999999949E+0002 T0s= 1119

t0= 1119

93)  $5\text{C}_2\text{H}_2 + 9\text{C}_2\text{H}_6 = 4\text{C}_7\text{H}_{16}$  180 734 88 409  
(sSfp-sSfl)=-3.24569999999367E+0002 T0s= -282

t0= -282

94)  $5\text{CH}_4 + 1\text{C}_7\text{H}_{16} = 6\text{C}_2\text{H}_6$  -122 325 -45 329  
(sSfp-sSfl)= 4.17999999970198E+0000 T0s= -18416

t0= -18416

95)  $5\text{C} + 8\text{C}_2\text{H}_6 = 3\text{C}_7\text{H}_{16}$  135 446 -162 307  
(sSfp-sSfl)=-1.38849999999627E+0002 T0s= -2136

t0= -2136

96)  $3\text{CH}_4 + 2\text{C}_2\text{H}_2 = 1\text{C}_7\text{H}_{16}$  45 230 54 102  
(sSfp-sSfl)=-1.27320000000065E+0002 T0s= 75

t0= 75

97)  $9\text{C} + 1\text{C}_7\text{H}_{16} = 8\text{C}_2\text{H}_2$  432 115 45 384  
(sSfp-sSfl)= 2.69381999999983E+0002 T0s= 1438

t0= 1438

98)  $3\text{C} + 4\text{CH}_4 = 1\text{C}_7\text{H}_{16}$  45 182 -72 102  
(sSfp-sSfl)=-7.99660000000149E+0001 T0s= -1456

t0= -1456

99)  $6\text{C}_4\text{H}_{10} + 1\text{C}_6\text{H}_{12} = 6\text{C}_5\text{H}_{12}$  -222 516 -210 493  
(sSfp-sSfl)=-2.32799999997951E+0001 T0s= 481

t0= 481

100)  $2\text{C}_4\text{H}_6 + 2\text{C}_5\text{H}_{12} = 3\text{C}_6\text{H}_{12}$  -88 300 -4 214  
(sSfp-sSfl)=-8.58200000000652E+0001 T0s= 983

t0= 983



(sSfp-sSfl)=-1.3613999999665E+0002 T0s= 1063

t0= 1063



(sSfp-sSfl)=-1.6739999999907E+0001 T0s= 234

t0= 234



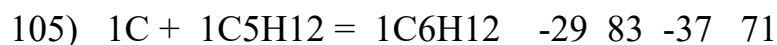
(sSfp-sSfl)=-2.81759999999311E+0002 T0s= 1095

t0= 1095



(sSfp-sSfl)=-2.97900000002701E+0001 T0s= -58

t0= -58



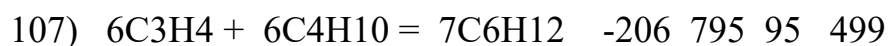
(sSfp-sSfl)=-1.22119999999413E+0001 T0s= -613

t0= -613



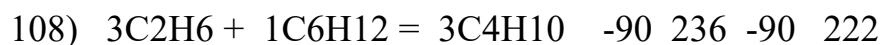
(sSfp-sSfl)=-1.40369999999646E+0002 T0s= 942

t0= 942



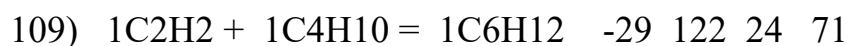
(sSfp-sSfl)=-2.95559999999125E+0002 T0s= 1017

t0= 1017



(sSfp-sSfl)=-1.34699999999721E+0001 T0s= 20

t0= 20



(sSfp-sSfl)=-5.08399999999674E+0001 T0s= 1048

t0= 1048



(sSfp-sSfl)=-1.21000000000931E+0001 T0s= -404



t0= -404

111)  $6C + 6C_4H_{10} = 5C_6H_{12}$  -147 453 -181 356

(sSfp-sSfl)=-9.65519999996759E+0001 T0s= -350

t0= -350

112)  $6C_3H_4 + 1C_6H_{12} = 6C_4H_6$  210 421 246 406

(sSfp-sSfl)=-1.48200000002980E+0001 T0s= 2447

t0= 2447

113)  $1C_2H_6 + 1C_4H_6 = 1C_6H_{12}$  -29 123 15 71

(sSfp-sSfl)=-5.12799999999115E+0001 T0s= 861

t0= 861

114)  $3C_2H_2 + 1C_6H_{12} = 3C_4H_6$  105 215 133 203

(sSfp-sSfl)=-1.21500000001397E+0001 T0s= 2281

t0= 2281

115)  $6CH_4 + 6C_4H_6 = 5C_6H_{12}$  -147 673 103 356

(sSfp-sSfl)=-3.17040000000037E+0002 T0s= 788

t0= 788

116)  $2C + 1C_6H_{12} = 2C_4H_6$  70 74 -29 135

(sSfp-sSfl)= 6.13959999999497E+0001 T0s= 1619

t0= 1619

117)  $6C_2H_6 + 6C_3H_4 = 5C_6H_{12}$  -147 679 154 356

(sSfp-sSfl)=-3.22500000000000E+0002 T0s= 934

t0= 934

118)  $6C_2H_2 + 1C_6H_{12} = 6C_3H_4$  276 359 295 350

(sSfp-sSfl)=-9.48000000044703E+0000 T0s= 2022

t0= 2022

119)  $3CH_4 + 3C_3H_4 = 2C_6H_{12}$  -59 308 84 143

(sSfp-sSfl)=-1.65930000000168E+0002 T0s= 862

t0= 862

120)  $3C + 1C_6H_{12} = 3C_3H_4$  138 75 -29 175

(sSfp-sSfl)= 9.95039999998407E+0001 T0s= 1680

t0= 1680



(sSfp-sSfl)=-1.6598999999758E+0002 T0s= 965

t0= 965



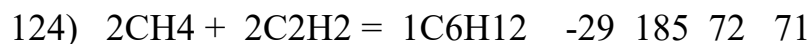
(sSfp-sSfl)=-9.36000000033528E+0000 T0s= -1625

t0= -1625



(sSfp-sSfl)=-4.11639999998733E+0001 T0s= -269

t0= -269



(sSfp-sSfl)=-1.13780000000028E+0002 T0s= 894

t0= 894



(sSfp-sSfl)= 2.08488000000012E+0002 T0s= 1696

t0= 1696



(sSfp-sSfl)=-6.64259999999776E+0001 T0s= -364

t0= -364



(sSfp-sSfl)=-7.78300000000745E+0001 T0s= 758

t0= 758



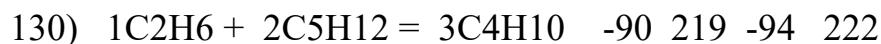
(sSfp-sSfl)=-3.27499999997672E+0001 T0s= 1009

t0= 1009



(sSfp-sSfl)=-7.64199999999255E+0001 T0s= 826

t0= 826



(sSfp-sSfl)= 3.27000000001863E+0000 T0s= 1113

t0= 1113



(sSfp-sSfl)=-7.41199999996461E+0001 T0s= 870

t0= 870



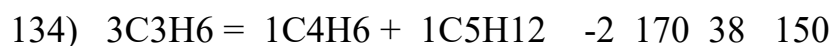
(sSfp-sSfl)= 5.58999999985099E+0000 T0s= 1438

t0= 1438



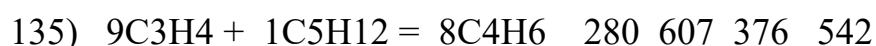
(sSfp-sSfl)=-3.54920000000857E+0001 T0s= 104

t0= 104



(sSfp-sSfl)=-2.04199999999255E+0001 T0s= 1967

t0= 1967



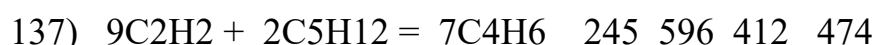
(sSfp-sSfl)=-6.51400000005960E+0001 T0s= 1483

t0= 1483



(sSfp-sSfl)=-6.80200000000186E+0001 T0s= 707

t0= 707



(sSfp-sSfl)=-1.22270000000484E+0002 T0s= 1370

t0= 1370



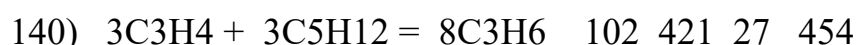
(sSfp-sSfl)=-2.61010000000242E+0002 T0s= 627

t0= 627



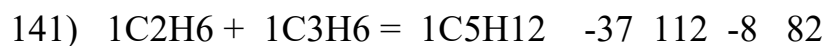
(sSfp-sSfl)= 4.91839999998920E+0001 T0s= 2173

t0= 2173



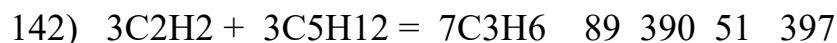
(sSfp-sSfl)= 3.27400000002235E+0001 T0s= 2288

t0= 2288



(sSfp-sSfl)=-2.9479999999814E+0001 T0s= 998

t0= 998



(sSfp-sSfl)= 6.89000000013039E+0000 T0s= 5498

t0= 5498



(sSfp-sSfl)=-1.14230000000214E+0002 T0s= 946

t0= 946



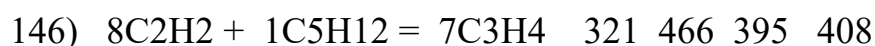
(sSfp-sSfl)= 3.00080000000307E+0001 T0s= 2079

t0= 2079



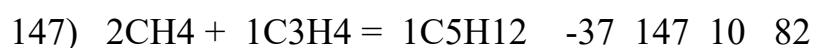
(sSfp-sSfl)=-2.03100000000093E+0002 T0s= 790

t0= 790



(sSfp-sSfl)=-5.80200000000186E+0001 T0s= 1272

t0= 1272



(sSfp-sSfl)=-6.52400000001071E+0001 T0s= 722

t0= 722



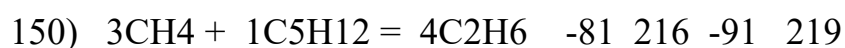
(sSfp-sSfl)= 8.72919999998994E+0001 T0s= 2001

t0= 2001



(sSfp-sSfl)=-1.99470000000205E+0002 T0s= 842

t0= 842



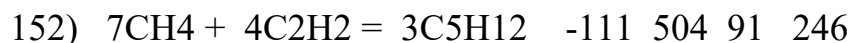
(sSfp-sSfl)= 3.68999999971129E+0000 T0s= 2591

t0= 2591



(sSfp-sSfl)=-2.89519999999320E+0001 T0s= -124

t0= -124



(sSfp-sSfl)=-2.57350000000326E+0002 T0s= 784

t0= 784



(sSfp-sSfl)= 1.96275999999954E+0002 T0s= 1839

t0= 1839



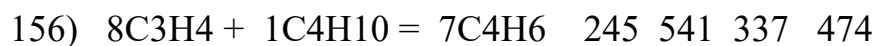
(sSfp-sSfl)=-5.42140000000363E+0001 T0s= -308

t0= -308



(sSfp-sSfl)=-2.85100000002421E+0001 T0s= 3068

t0= 3068



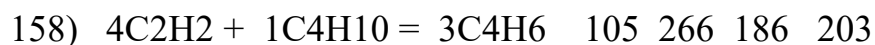
(sSfp-sSfl)=-6.65499999998137E+0001 T0s= 1389

t0= 1389



(sSfp-sSfl)=-6.47499999997672E+0001 T0s= 686

t0= 686



(sSfp-sSfl)=-6.29900000002235E+0001 T0s= 1286

t0= 1286



(sSfp-sSfl)=-1.88770000000019E+0002 T0s= 597

t0= 597



(sSfp-sSfl)= 1.05213999999920E+0002 T0s= 2522

t0= 2522

161)  $3C_3H_4 + 3C_4H_{10} = 7C_3H_6$  89 397 47 397  
(sSfp-sSfl)=-9.99999977648258E-0003 T0s=-4187000

t0=-4187000

162)  $3C_2H_6 + 2C_3H_6 = 3C_4H_{10}$  -90 278 -35 222  
(sSfp-sSfl)=-5.56900000001770E+0001 T0s= 991

t0= 991

163)  $1C_2H_2 + 1C_4H_{10} = 2C_3H_6$  25 122 24 114  
(sSfp-sSfl)=-8.61999999999534E+0000 T0s= -187

t0= -187

164)  $1CH_4 + 1C_3H_6 = 1C_4H_{10}$  -30 101 -5 74  
(sSfp-sSfl)=-2.71600000000326E+0001 T0s= 921

t0= 921

165)  $3C + 3C_4H_{10} = 5C_3H_6$  64 226 -90 284  
(sSfp-sSfl)= 5.72739999999758E+0001 T0s= 2691

t0= 2691

166)  $7C_2H_6 + 2C_3H_4 = 5C_4H_{10}$  -151 501 -50 371  
(sSfp-sSfl)=-1.29949999999721E+0002 T0s= 776

t0= 776

167)  $7C_2H_2 + 1C_4H_{10} = 6C_3H_4$  276 410 348 350  
(sSfp-sSfl)=-6.03200000002980E+0001 T0s= 1201

t0= 1201

168)  $7CH_4 + 3C_3H_4 = 4C_4H_{10}$  -121 487 13 296  
(sSfp-sSfl)=-1.90130000000354E+0002 T0s= 701

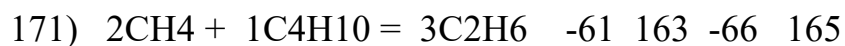
t0= 701

169)  $7C + 2C_4H_{10} = 5C_3H_4$  230 158 -60 292  
(sSfp-sSfl)= 1.33655999999959E+0002 T0s= 2169

t0= 2169

170)  $1C_2H_2 + 3C_2H_6 = 2C_4H_{10}$  -60 213 -7 148  
(sSfp-sSfl)=-6.43100000000559E+0001 T0s= 833

t0= 833



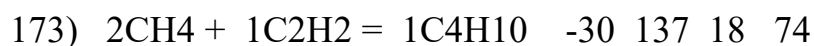
(sSfp-sSfl)= 1.36999999987893E+0000 T0s= 3766

t0= 3766



(sSfp-sSfl)=-5.46339999998454E+0001 T0s= -198

t0= -198



(sSfp-sSfl)=-6.29400000000605E+0001 T0s= 769

t0= 769



(sSfp-sSfl)= 1.57648000000045E+0002 T0s= 1905

t0= 1905



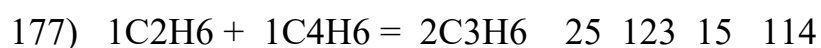
(sSfp-sSfl)=-7.85260000000708E+0001 T0s= -371

t0= -371



(sSfp-sSfl)=-2.85200000000186E+0001 T0s= 1599

t0= 1599



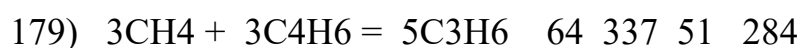
(sSfp-sSfl)=-9.05999999993946E+0000 T0s= -1188

t0= -1188



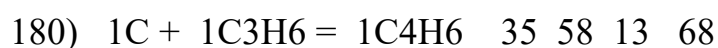
(sSfp-sSfl)=-5.43700000001118E+0001 T0s= 1520

t0= 1520



(sSfp-sSfl)=-5.29700000002049E+0001 T0s= -235

t0= -235



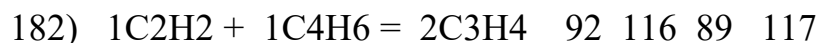
(sSfp-sSfl)= 9.58799999998882E+0000 T0s= 2319

t0= 2319



(sSfp-sSfl)=-6.6100000000931E+0001 T0s= 1217

t0= 1217



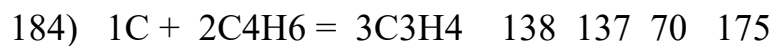
(sSfp-sSfl)= 8.90000000013970E-0001 T0s= 3202

t0= 3202



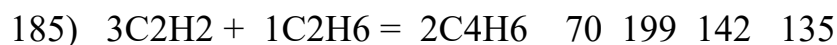
(sSfp-sSfl)=-6.5189999999441E+0001 T0s= 1102

t0= 1102



(sSfp-sSfl)= 3.81080000000075E+0001 T0s= 1780

t0= 1780



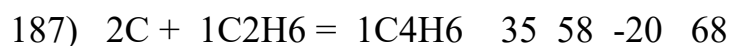
(sSfp-sSfl)=-6.34300000001676E+0001 T0s= 1133

t0= 1133



(sSfp-sSfl)=-6.06400000001304E+0001 T0s= 477

t0= 477



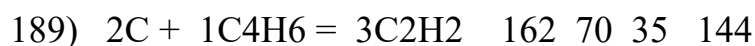
(sSfp-sSfl)= 1.01159999999800E+0001 T0s= 5459

t0= 5459



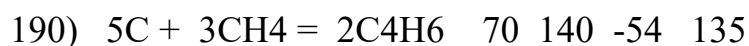
(sSfp-sSfl)=-1.25930000000168E+0002 T0s= 1028

t0= 1028



(sSfp-sSfl)= 7.35460000000894E+0001 T0s= 1728

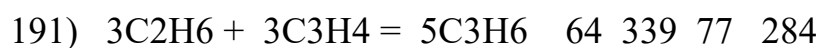
t0= 1728



(sSfp-sSfl)=-5.03000000026077E+0000 T0s= -24569



t0= -24569



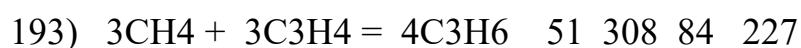
(sSfp-sSfl)=-5.57000000001863E+0001 T0s= 239

t0= 239



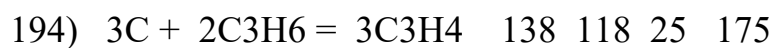
(sSfp-sSfl)=-2.58500000000931E+0001 T0s= 1433

t0= 1433



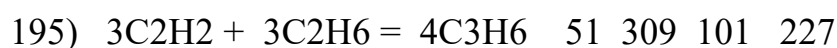
(sSfp-sSfl)=-8.14900000002235E+0001 T0s= 407

t0= 407



(sSfp-sSfl)= 5.72839999998687E+0001 T0s= 1960

t0= 1960



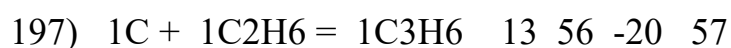
(sSfp-sSfl)=-8.15499999998137E+0001 T0s= 617

t0= 617



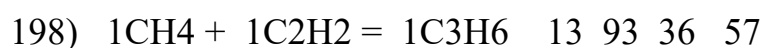
(sSfp-sSfl)=-2.57900000000373E+0001 T0s= 770

t0= 770



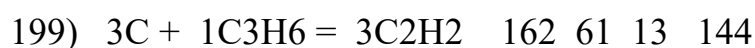
(sSfp-sSfl)= 5.28000000049360E-0001 T0s= 62481

t0= 62481



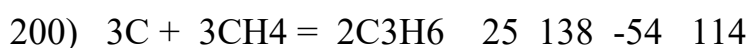
(sSfp-sSfl)=-3.57800000000279E+0001 T0s= 654

t0= 654



(sSfp-sSfl)= 8.31340000000200E+0001 T0s= 1796

t0= 1796



(sSfp-sSfl)=-2.42060000000056E+0001 T0s= -3269

t0= -3269



(sSfp-sSfl)=-6.16500000001397E+0001 T0s= 1073

t0= 1073



(sSfp-sSfl)=-6.15500000002794E+0001 T0s= 610

t0= 610



(sSfp-sSfl)= 5.83399999999674E+0001 T0s= 3056

t0= 3056



(sSfp-sSfl)=-6.16300000001211E+0001 T0s= 981

t0= 981



(sSfp-sSfl)= 3.63280000000377E+0001 T0s= 1710

t0= 1710



(sSfp-sSfl)= 1.10259999999544E+0001 T0s= 5786

t0= 5786



(sSfp-sSfl)=-6.15700000000652E+0001 T0s= 702

t0= 702



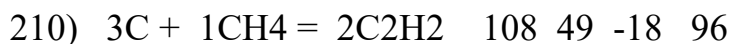
(sSfp-sSfl)= 8.36620000000112E+0001 T0s= 2179

t0= 2179



(sSfp-sSfl)=-2.52620000001043E+0001 T0s= -520

t0= -520



(sSfp-sSfl)= 4.7353999999921E+0001 T0s= 2659

t0= 2659

211)  $26C6H12 = 18C7H16 + 3C10H8$  864 1853 -765 1961

(sSfp-sSfl)= 1.07250000000000E+0002 T0s= 15189

t0= 15189

Список завершен

Сортировка и выбор группы базовых реакций

196 18 420 190 412 416 14 400 164 380

192 182 154 348 252 160 122 306 178 186

6 140 118 406 308 4 142 112 146 150

128 110 132 136 250 174 350 170 130 144

108 398 374 137 119 338 394 151 133 296

86 115 2 422 102 378 104 123 97 171

418 147 246 113 61 47 94 320 50 31

34 194 240 66 64 83 167 10 278 73

76 52 175 161 410 90 82 156 330 388

15 91 302 187 36 125 57 100 43 72

Порядковые номера реакций в группе с max потенциалом:

196 18 420 190 412 400 164 154 252 306

-98 -9 -210 -95 -206 -200 -82 -77 -126 -153

Термодинамический потенциал суммарный в указанных ед.

dgs= -1334.958

Список линейно независимых реакций

- 98)  $3C + 4CH4 = 1C7H16$  45 182 -72 102

(sSfp-sSfl)=-7.99660000000149E+0001 T0s= -1456

- 9)  $26CH4 + 3C10H8 = 8C7H16$  359 1277 -409 818

(sSfp-sSfl)=-4.59290000000969E+0002 T0s= -1672

- 210)  $3C + 1CH4 = 2C2H2$  108 49 -18 96

(sSfp-sSfl)= 4.7353999999921E+0001 T0s= 2659

- 95)  $5C + 8C2H6 = 3C7H16$  135 446 -162 307

(sSfp-sSfl)=-1.3884999999627E+0002 T0s= -2136

- 206) 2C + 1CH4 = 1C3H4 46 47 -18 58

(sSfp-sSfl)= 1.1025999999544E+0001 T0s= 5786

- 200) 3C + 3CH4 = 2C3H6 25 138 -54 114

(sSfp-sSfl)=-2.42060000000056E+0001 T0s= -3269

- 82) 11CH4 + 6C4H6 = 5C7H16 224 896 13 511

(sSfp-sSfl)=-3.84740000000689E+0002 T0s= -549

- 77) 3C + 8C4H10 = 5C7H16 224 597 -241 511

(sSfp-sSfl)=-8.57260000002570E+0001 T0s= -5431

- 126) 3C + 3CH4 = 1C6H12 -29 138 -54 71

(sSfp-sSfl)=-6.6425999999776E+0001 T0s= -364

- 153) 7C + 1C5H12 = 6C2H2 324 92 -37 288

(sSfp-sSfl)= 1.9627599999954E+0002 T0s= 1839

1C7H16+8C7H16+2C2H2+3C7H16+1C3H4+2C3H6+5C7H16+5C7H16+  
1C6H12+6C2H2=

3C + 4CH4+26CH4 + 3C10H8+3C + 1CH4+5C + 8C2H6+2C + 1CH4+

3C + 3CH4+11CH4 + 6C4H6+3C + 8C4H10+3C + 3CH4+7C + 1C5H12

Баланс элементов

185=185 C

396=396 H

В списке линейно независимых реакций есть условные отрицательные температуры T0, и прямая для приблизительного расчета энергии Гиббса направлена вверх. Это значит, данная реакция не выполнима в рассматриваемом диапазоне температур. Рассчитаем точно энергию Гиббса на примере реакции

129) 7C + 8H2O = 4O2 + 1C7H16 45 370 -462 298

(sSfp-sSfl)=-7.2162000000112E+0001 T0s= -7029

Program BENZ(f1,f2,f3,f4,f5,f6);

{Calculation of Gibbs energy change 7C+8H2O=4O2+1C7H16}

const a=-72.162; b=507248;

var dgg,dg,T,C,H2O,O2,C7H16,dgg0:real;

```

f1,f2,f3,f4,f5,f6:text;

begin
assign(f1,'c:\max\text\t.t');
assign(f2,'c:\max\text\dgd.pas');
assign(f3,'c:\max\text\GTC.t');
assign(f4,'c:\max\text\GTH2O.t');
assign(f5,'c:\max\text\GTO2.t');
assign(f6,'c:\max\text\GTC7H16.t');
reset(f1); rewrite(f2); reset(f3); reset(f4); reset(f5); reset(f6);
{dgg0:= (4.85599400000095E+0005 +4.10725938952565E+0004);}
while EOF(f1)=false do begin
    readln(f1,T);
    dgg:=a*T+b;
readln(f3,C); readln(f4,H2O); readln(f5,O2); readln(f6,C7H16);
dg:=- (7*C+8*H2O)+(4*O2+1*C7H16){+dgg0};
    writeln(f2,dgg,' ',dg{' ',T});
    end;

close(f1);close(f2);close(f3);close(f4);close(f5);close(f6);

```

На рис. 1 можно видеть то, что в этом случае уточненная величина энергии Гиббса отличается от прямой линии по температуре и реакция осуществима только при температурах выше  $T_0$ . Обратная реакция при  $T=1000$  К протекает.

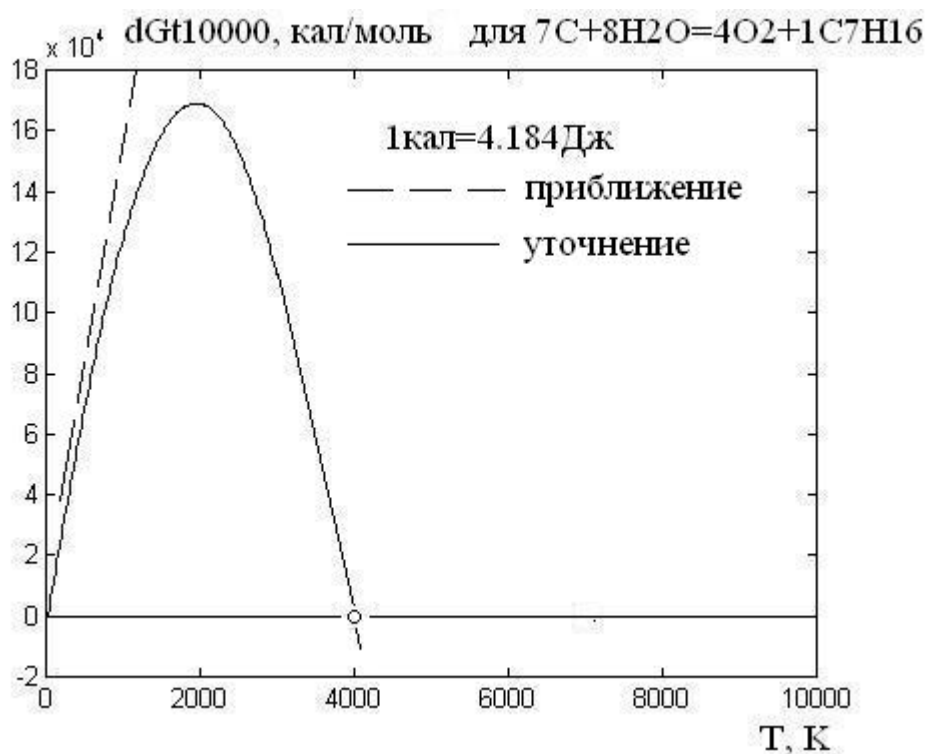


Рис. 1

В правой части уравнения суммарной реакции мы имеем вещества:  
C, CH<sub>4</sub>, C<sub>10</sub>H<sub>8</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>4</sub>H<sub>6</sub>, C<sub>4</sub>H<sub>10</sub>, C<sub>5</sub>H<sub>12</sub>.

Можно проверить, как эти вещества реагируют между собой.

Начальные данные

$n_b = 2$   $n_p = 7$   $t_k = 1000$  К

Атомные веса элементов:

12.00 1.01

Наименования веществ dhf, ккал/моль s0, кал/мольК

C	0.000	1.372
CH <sub>4</sub>	-17.880	44.530
C <sub>2</sub> H <sub>6</sub>	-20.250	54.850
C <sub>4</sub> H <sub>6</sub>	34.970	67.710
C <sub>4</sub> H <sub>10</sub>	-30.150	74.120
C <sub>5</sub> H <sub>12</sub>	-36.920	82.120
C <sub>10</sub> H <sub>8</sub>	18.660	39.890

Матрица групп элементов в веществах

1.0 0.0

1.0 4.0

2.0 6.0

4.0 6.0

4.0 10.0

5.0 12.0

10.0 8.0

#### Расчетные данные

1)  $40C_4H_{10} + 1C_{10}H_8 = 34C_5H_{12}$  -1255 3005 -1187 2792

(sSfp-sSfl)=-2.12610000003129E+0002 T0s= 320

t0= 320

2)  $40C_4H_6 = 14C_5H_{12} + 9C_{10}H_8$  -349 2708 1399 1509

(sSfp-sSfl)=-1.19970999999903E+0003 T0s= 1457

t0= 1457

3)  $40C_2H_6 + 3C_{10}H_8 = 22C_5H_{12}$  -812 2314 -754 1807

(sSfp-sSfl)=-5.07030000001192E+0002 T0s= 115

t0= 115

4)  $10CH_4 + 1C_{10}H_8 = 4C_5H_{12}$  -148 485 -160 328

(sSfp-sSfl)=-1.56710000000428E+0002 T0s= -80

t0= -80

5)  $20C + 2C_5H_{12} = 3C_{10}H_8$  56 192 -74 120

(sSfp-sSfl)=-7.20099999998929E+0001 T0s= -1803

t0= -1803

6)  $17C_4H_6 = 7C_4H_{10} + 4C_{10}H_8$  -136 1151 594 678

(sSfp-sSfl)=-4.7266999999925E+0002 T0s= 1546

t0= 1546

7)  $17C_2H_6 + 1C_{10}H_8 = 11C_4H_{10}$  -332 972 -326 815

(sSfp-sSfl)=-1.57019999998622E+0002 T0s= 39

t0= 39

8)  $34CH_4 + 3C_{10}H_8 = 16C_4H_{10}$  -482 1634 -552 1186

(sSfp-sSfl)=-4.47770000001416E+0002 T0s= -155

t0= -155

9)  $34C + 4C_4H_{10} = 5C_{10}H_8$  93 343 -121 199

(sSfp-sSfl)=-1.43677999999840E+0002 T0s= -1489

t0= -1489

10)  $7C_2H_6 + 3C_{10}H_8 = 11C_4H_6$  385 504 -86 745

(sSfp-sSfl)= 2.41189999999944E+0002 T0s= 1950

t0= 1950

11)  $14CH_4 + 5C_{10}H_8 = 16C_4H_6$  560 823 -157 1083

(sSfp-sSfl)= 2.60489999998361E+0002 T0s= 2751

t0= 2751

12)  $14C + 4C_4H_6 = 3C_{10}H_8$  56 290 140 120

(sSfp-sSfl)=-1.70377999999910E+0002 T0s= 492

t0= 492

13)  $22CH_4 + 1C_{10}H_8 = 16C_2H_6$  -324 1020 -375 878

(sSfp-sSfl)=-1.41950000001118E+0002 T0s= -357

t0= -357

14)  $22C + 4C_2H_6 = 3C_{10}H_8$  56 250 -81 120

(sSfp-sSfl)=-1.29913999999757E+0002 T0s= -1054

t0= -1054

15)  $8C + 2CH_4 = 1C_{10}H_8$  19 100 -36 40

(sSfp-sSfl)=-6.01460000000661E+0001 T0s= -905

t0= -905

16)  $1C_4H_6 + 9C_4H_{10} = 8C_5H_{12}$  -295 735 -236 657

(sSfp-sSfl)=-7.78300000000745E+0001 T0s= 758

t0= 758

17)  $1C_2H_6 + 2C_5H_{12} = 3C_4H_{10}$  -90 219 -94 222

(sSfp-sSfl)= 3.27000000001863E+0000 T0s= 1113

t0= 1113

18)  $1CH_4 + 3C_5H_{12} = 4C_4H_{10}$  -121 291 -129 296

(sSfp-sSfl)= 5.58999999985099E+0000 T0s= 1438



t0= 1438

19)  $1C + 6C_4H_{10} = 5C_5H_{12}$  -185 446 -181 411  
(sSfp-sSfl)=-3.54920000000857E+0001 T0s= 104

t0= 104

20)  $3C_2H_6 + 1C_4H_6 = 2C_5H_{12}$  -74 232 -26 164  
(sSfp-sSfl)=-6.80200000000186E+0001 T0s= 707

t0= 707

21)  $9CH_4 + 4C_4H_6 = 5C_5H_{12}$  -185 672 -21 411  
(sSfp-sSfl)=-2.61010000000242E+0002 T0s= 627

t0= 627

22)  $3C + 1C_5H_{12} = 2C_4H_6$  70 86 -37 135  
(sSfp-sSfl)= 4.91839999998920E+0001 T0s= 2173

t0= 2173

23)  $3CH_4 + 1C_5H_{12} = 4C_2H_6$  -81 216 -91 219  
(sSfp-sSfl)= 3.68999999971129E+0000 T0s= 2591

t0= 2591

24)  $1C + 2C_2H_6 = 1C_5H_{12}$  -37 111 -41 82  
(sSfp-sSfl)=-2.89519999999320E+0001 T0s= -124

t0= -124

25)  $2C + 3CH_4 = 1C_5H_{12}$  -37 136 -54 82  
(sSfp-sSfl)=-5.42140000000363E+0001 T0s= -308

t0= -308

26)  $4C_2H_6 + 1C_4H_6 = 3C_4H_{10}$  -90 287 -46 222  
(sSfp-sSfl)=-6.47499999997672E+0001 T0s= 686

t0= 686

27)  $8CH_4 + 3C_4H_6 = 5C_4H_{10}$  -151 559 -38 371  
(sSfp-sSfl)=-1.88770000000019E+0002 T0s= 597

t0= 597

28)  $8C + 3C_4H_{10} = 5C_4H_6$  175 233 -90 339  
(sSfp-sSfl)= 1.05213999999920E+0002 T0s= 2522

t0= 2522

29)  $2\text{CH}_4 + 1\text{C}_4\text{H}_{10} = 3\text{C}_2\text{H}_6$  -61 163 -66 165  
(sSfp-sSfl)= 1.36999999987893E+0000 T0s= 3766

t0= 3766

30)  $2\text{C} + 5\text{C}_2\text{H}_6 = 3\text{C}_4\text{H}_{10}$  -90 277 -101 222  
(sSfp-sSfl)=-5.46339999998454E+0001 T0s= -198

t0= -198

31)  $3\text{C} + 5\text{CH}_4 = 2\text{C}_4\text{H}_{10}$  -60 227 -89 148  
(sSfp-sSfl)=-7.85260000000708E+0001 T0s= -371

t0= -371

32)  $6\text{CH}_4 + 1\text{C}_4\text{H}_6 = 5\text{C}_2\text{H}_6$  -101 335 -72 274  
(sSfp-sSfl)=-6.06400000001304E+0001 T0s= 477

t0= 477

33)  $2\text{C} + 1\text{C}_2\text{H}_6 = 1\text{C}_4\text{H}_6$  35 58 -20 68  
(sSfp-sSfl)= 1.01159999999800E+0001 T0s= 5459

t0= 5459

34)  $5\text{C} + 3\text{CH}_4 = 2\text{C}_4\text{H}_6$  70 140 -54 135  
(sSfp-sSfl)=-5.03000000026077E+0000 T0s= -24569

t0= -24569

35)  $1\text{C} + 3\text{CH}_4 = 2\text{C}_2\text{H}_6$  -41 135 -54 110  
(sSfp-sSfl)=-2.52620000001043E+0001 T0s= -520

t0= -520

36)  $40\text{C}_4\text{H}_{10} + 1\text{C}_{10}\text{H}_8 = 34\text{C}_5\text{H}_{12}$  -1255 3005 -1187 2792  
(sSfp-sSfl)=-2.12610000003129E+0002 T0s= 320

t0= 320

Список завершен

Сортировка и выбор группы базовых реакций

68 50 62 30 66 28 70 56 8 18

16 44 22 10 48 26 20 60 6 11

42 54 3 14 24 64 40 52 38 2

72 46 58 32 36 34 33 35 31 57  
 45 1 71 37 51 39 63 23 13 4  
 53 41 12 5 59 19 25 47 9 21  
 43 15 17 7 55 69 27 65 29 61  
 49 67 67 67 67 67 67 67 67 67  
 67 67 67 67 67 67 67 67 67 67  
 67 67 67 67 67 67 67 67 67 67

Порядковые номера реакций в группе с max потенциалом:

68 50 62 30 66  
 -34 -25 -31 -15 -33

Термодинамический потенциал суммарный в указанных ед.

dgs= -975.706  
 - 34)  $5C + 3CH_4 = 2C_4H_6$  70 140 -54 135  
 - 25)  $2C + 3CH_4 = 1C_5H_{12}$  -37 136 -54 82  
 - 31)  $3C + 5CH_4 = 2C_4H_{10}$  -60 227 -89 148  
 - 15)  $8C + 2CH_4 = 1C_{10}H_8$  19 100 -36 40  
 - 33)  $2C + 1C_2H_6 = 1C_4H_6$  35 58 -20 68

Далее в правой части C, CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>.

Начальные данные

nb= 2 np= 3 tk=1000 K

Атомные веса элементов:

12.00 1.01

Наименования веществ dhf, ккал/моль s0, кал/ мольК

C	0.000	1.372
CH <sub>4</sub>	-17.880	44.530
C <sub>2</sub> H <sub>6</sub>	-20.250	54.850

Матрица групп элементов в веществах

1.0	0.0
1.0	4.0
2.0	6.0

Расчетные данные



$(sSfp-sSfl)=-2.52620000001043E+0001$   $T0s= -520$

$t0= -520$



$(sSfp-sSfl)=-2.52620000001043E+0001$   $T0s= -520$

$t0= -520$

Список завершен

Сортировка и выбор группы базовых реакций

2 4 1 3 3 3 3 3 3 3

3 3 3 3 3 3 3 3 3 3

3 3 3 3 3 3 3 3 3 3

3 3 3 3 3 3 3 3 3 3

3 3 3 3 3 3 3 3 3 3

3 3 3 3 3 3 3 3 3 3

3 3 3 3 3 3 3 3 3 3

3 3 3 3 3 3 3 3 3 3

3 3 3 3 3 3 3 3 3 3

3 3 3 3 3 3 3 3 3 3

Порядковые номера реакций в группе с max потенциалом:

2

-1

Термодинамический потенциал суммарный в указанных ед.

$dgs= -639.011$



В правой части остаются только углерод и метан.

*Список литературы*

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