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# Thermal Decomposition Kinetics of Light Polycyclic Aromatic Hydrocarbons as Surrogate Biomass Tar

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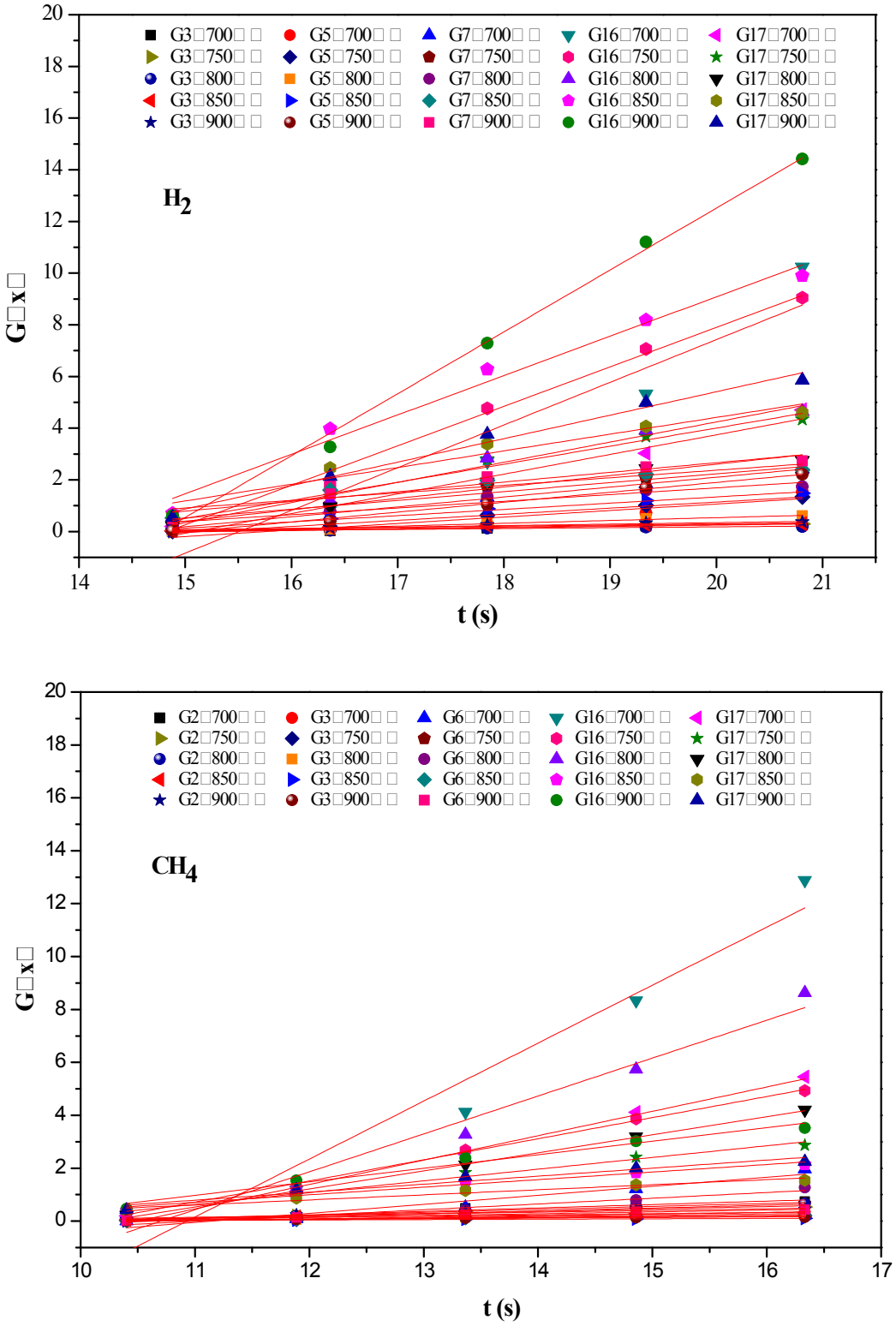
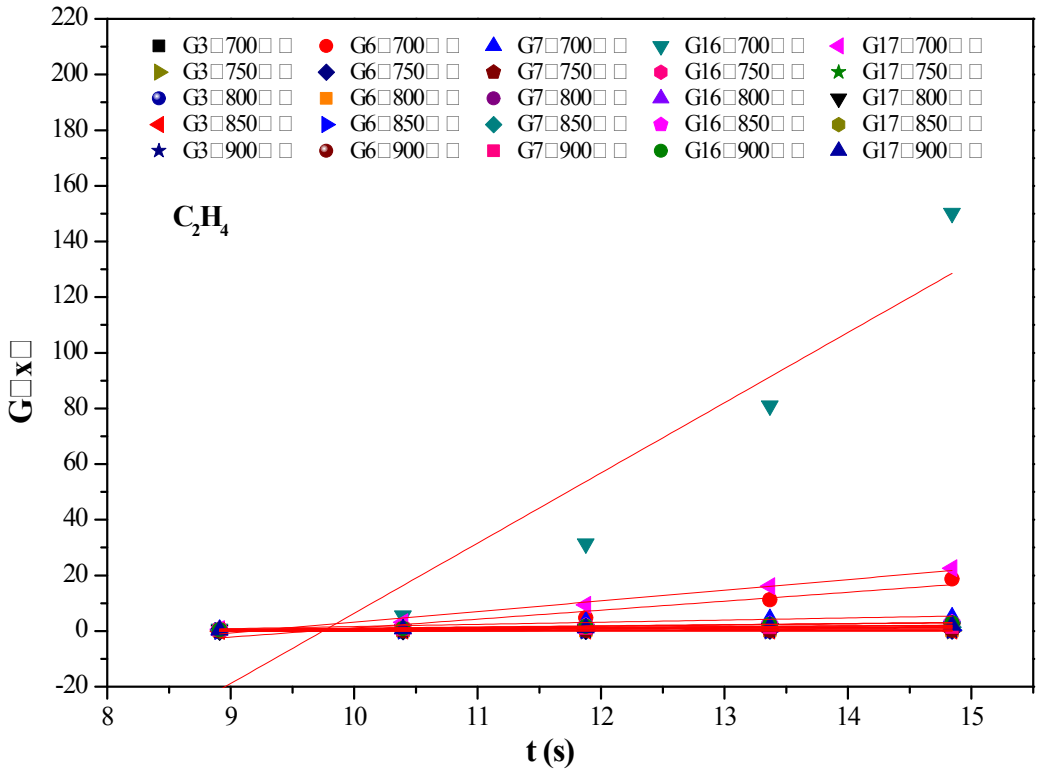
**Fig.S1.** Correlation of G(X) versus t at different reaction temperatures for individual gas component from the thermal decomposition of naphthalene.

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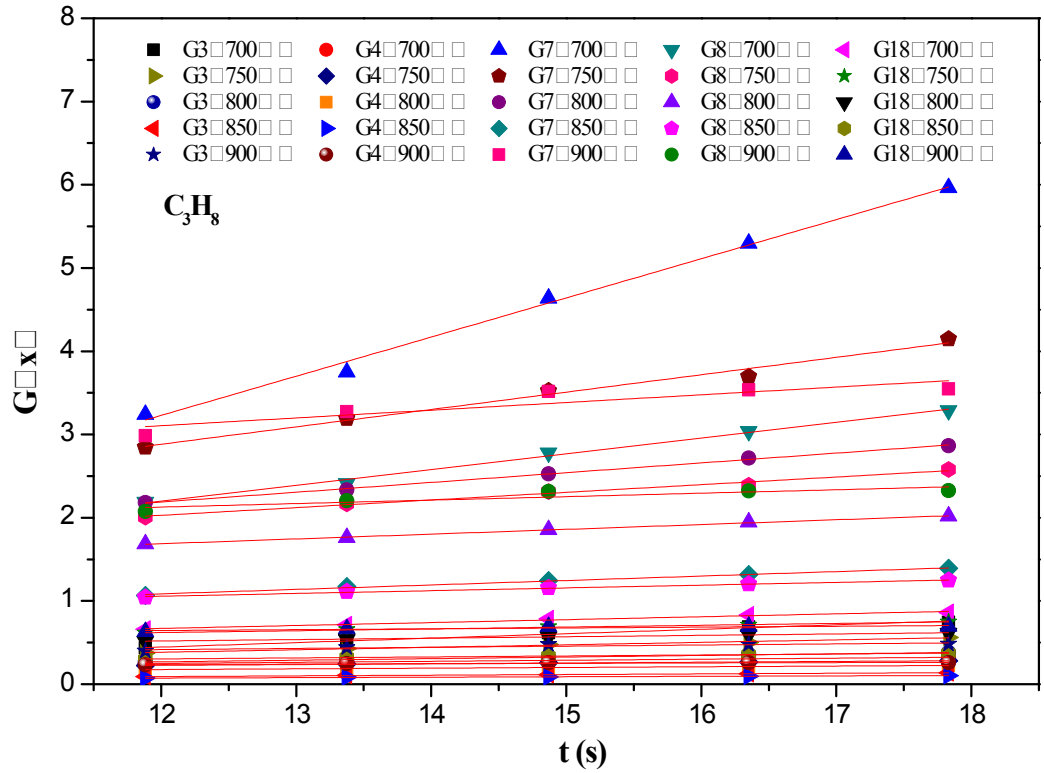
C2H4
G□x□
t (s)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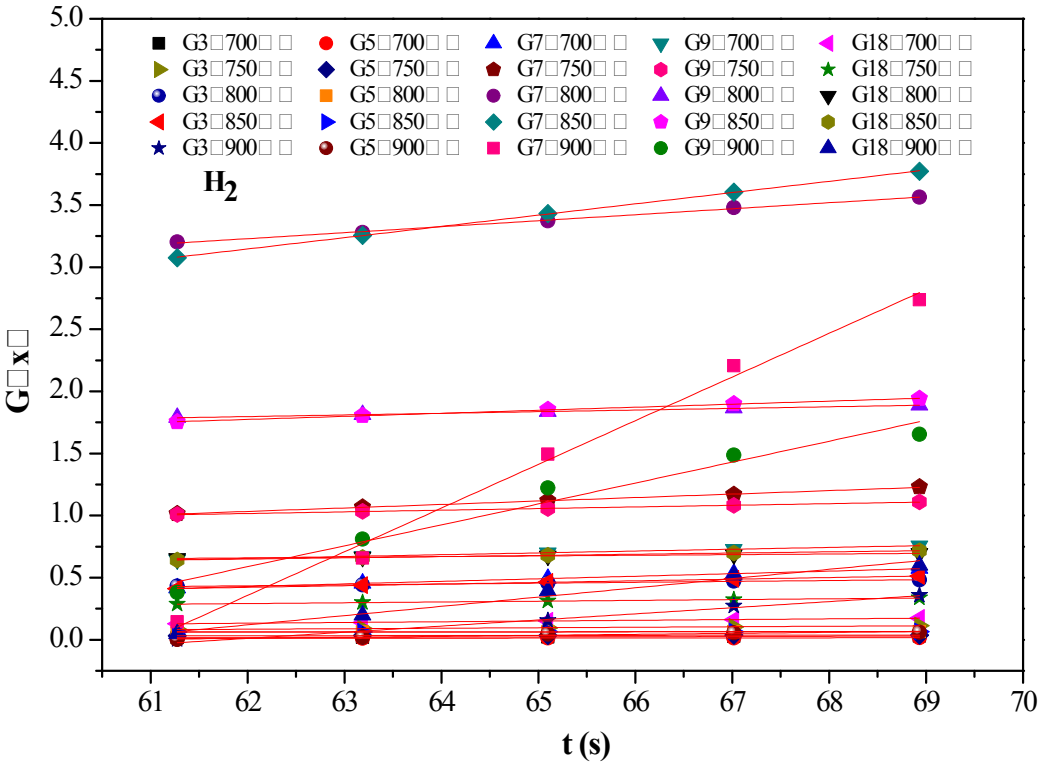
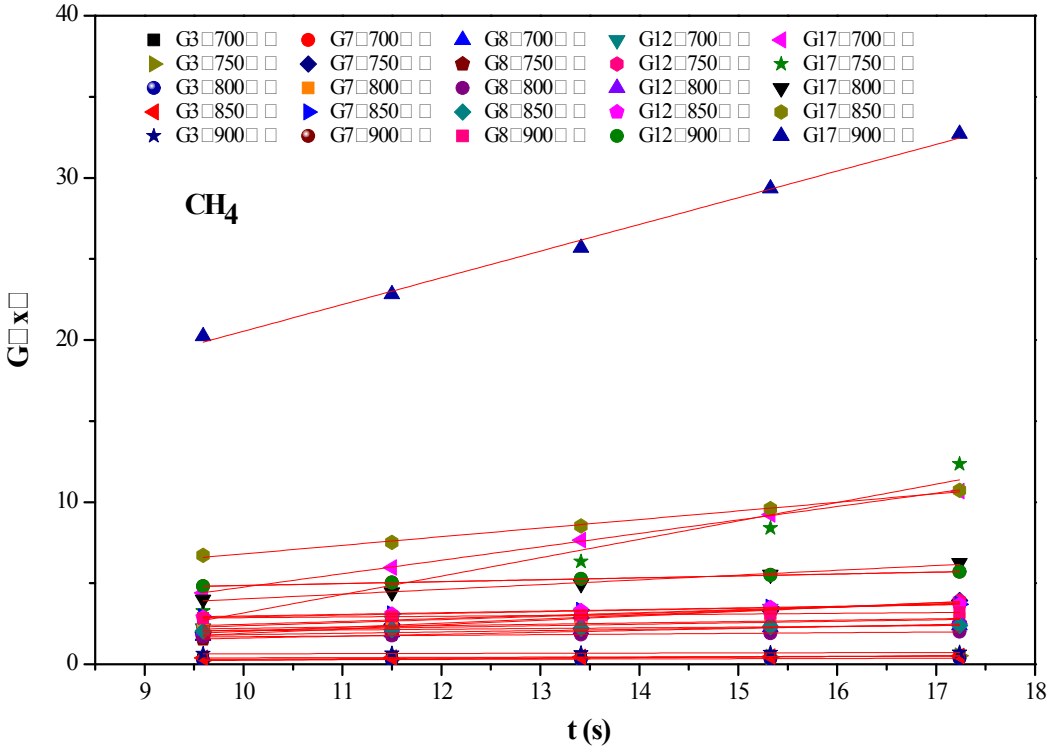
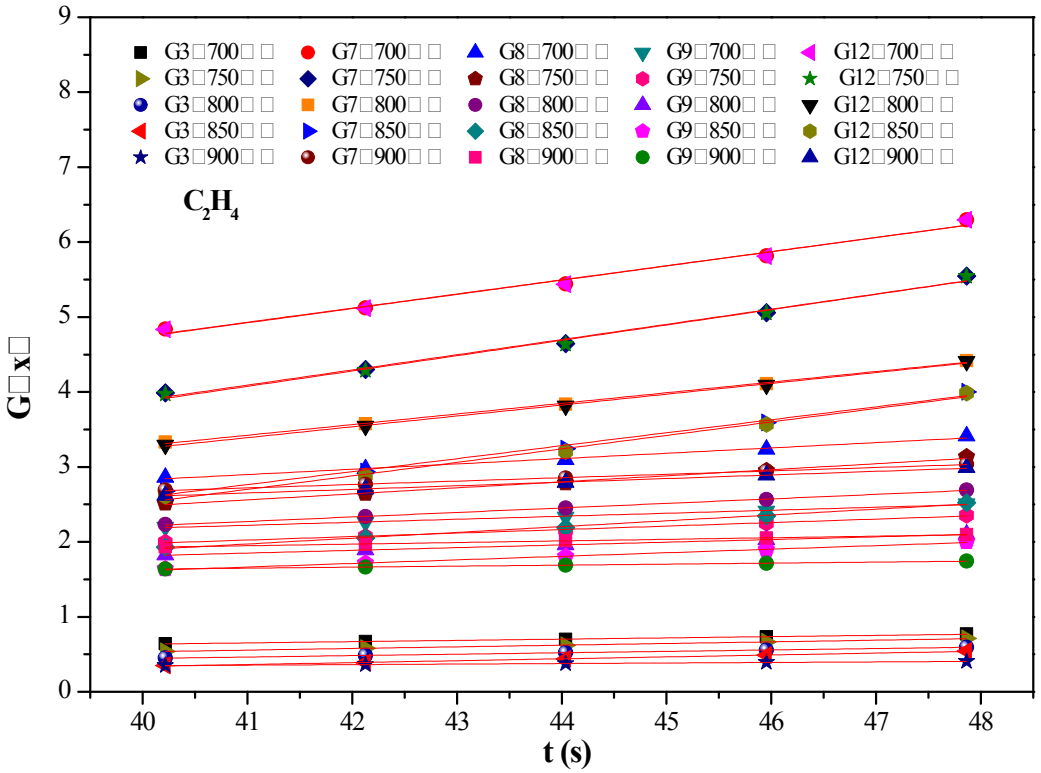
G18□900□□
C3H8
G□x□
t (s)

**Fig.S2.** Correlation of G(X) versus t at different reaction temperatures for individual gas component from the thermal decomposition of anthracene.

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G7□900□□
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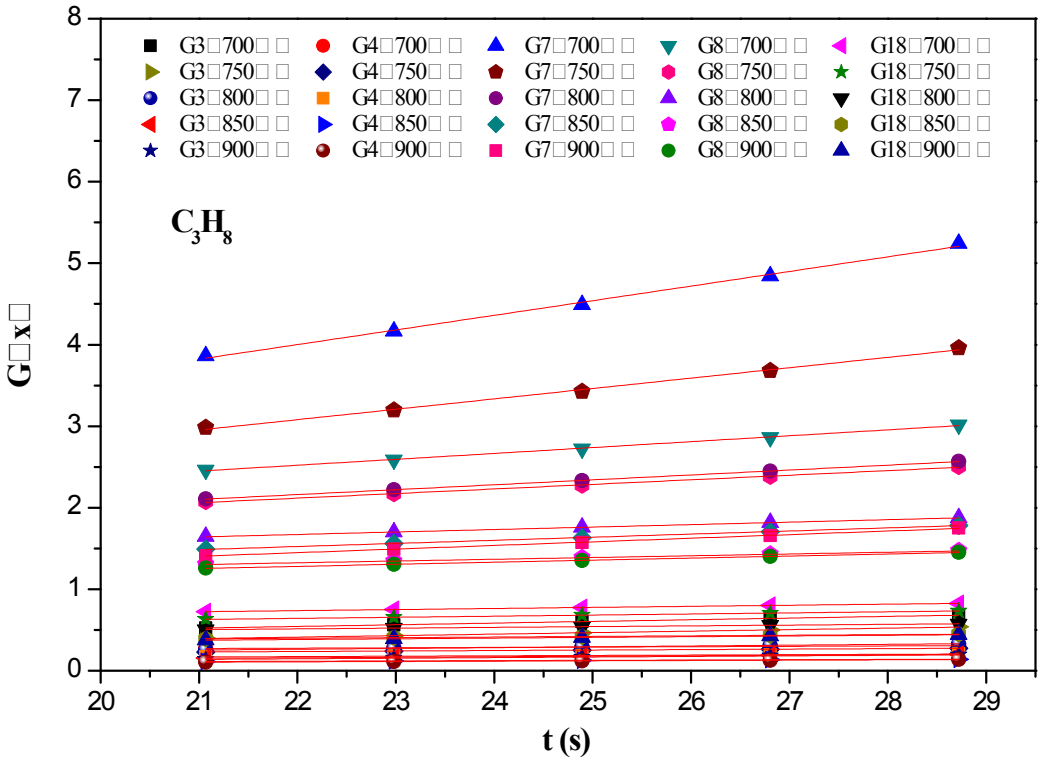
G12□900□□
C2H4
G□x□
t (s)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G18□700□□
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G4□900□□
G7□900□□
G8□900□□
G18□900□□
C3H8
G□x□
t (s)

**Table S1** Apparent activation energies of individual gas component during the thermal decomposition of naphthalene and anthracene.

| Individual gas | Conversion fraction (%) | Naphthalene | | | Anthracene | | |
|---|---|---|---|---|---|---|---|
| | | $E_a$ | SD | $R^2$ | $E_a$ | SD | $R^2$ |
| $H_2$ | 20 | 26.9 | 0.048 | 0.902 | 89.6 | 0.047 | 0.922 |
| | 30 | 27.4 | 0.043 | 0.913 | 114.5 | 0.039 | 0.933 |
| | 40 | 28.1 | 0.039 | 0.932 | 132.8 | 0.023 | 0.952 |
| | 50 | 29.5 | 0.035 | 0.945 | 152.0 | 0.022 | 0.967 |
| | 60 | 31.7 | 0.036 | 0.957 | 167.6 | 0.031 | 0.968 |
| | 70 | 43.2 | 0.044 | 0.933 | 167.7 | 0.040 | 0.947 |
| | 80 | 57.6 | 0.039 | 0.921 | 167.9 | 0.037 | 0.939 |
| | Average/(kJ/mol) | 34.9 | | | 141.7 | | |
| $CH_4$ | 20 | 42.7 | 0.049 | 0.912 | 46.5 | 0.049 | 0.913 |
| | 30 | 46.9 | 0.044 | 0.923 | 47.8 | 0.048 | 0.922 |
| | 40 | 47.9 | 0.042 | 0.942 | 48.5 | 0.042 | 0.945 |
| | 50 | 48.9 | 0.039 | 0.955 | 50.4 | 0.038 | 0.965 |
| | 60 | 49.8 | 0.034 | 0.967 | 54.7 | 0.037 | 0.965 |
| | 70 | 54.8 | 0.041 | 0.943 | 61.5 | 0.040 | 0.946 |
| | 80 | 55.9 | 0.039 | 0.931 | 91.5 | 0.041 | 0.933 |
| | Average/(kJ/mol) | 49.5 | | | 57.3 | | |
| $C_2H_4$ | 20 | 35.9 | 0.043 | 0.921 | 45.9 | 0.041 | 0.911 |
| | 30 | 37.8 | 0.037 | 0.932 | 55.3 | 0.038 | 0.923 |
| | 40 | 39.5 | 0.032 | 0.956 | 65.9 | 0.034 | 0.932 |
| | 50 | 41.8 | 0.021 | 0.967 | 78.3 | 0.029 | 0.955 |
| | 60 | 49.2 | 0.030 | 0.968 | 95.8 | 0.028 | 0.957 |
| | 70 | 58.7 | 0.034 | 0.945 | 114.5 | 0.034 | 0.943 |
| | 80 | 75.1 | 0.038 | 0.937 | 135.9 | 0.038 | 0.921 |
| | Average/(kJ/mol) | 48.3 | | | 84.5 | | |
| $C_3H_8$ | 20 | 16.7 | 0.042 | 0.924 | 43.8 | 0.042 | 0.914 |
| | 30 | 17.3 | 0.037 | 0.942 | 45.2 | 0.038 | 0.925 |
| | 40 | 19.7 | 0.032 | 0.936 | 51.2 | 0.035 | 0.932 |
| | 50 | 21.1 | 0.023 | 0.967 | 58.8 | 0.029 | 0.955 |
| | 60 | 24.5 | 0.030 | 0.988 | 69.1 | 0.028 | 0.959 |
| | 70 | 33.5 | 0.037 | 0.945 | 82.7 | 0.035 | 0.943 |
| | 80 | 49.8 | 0.038 | 0.947 | 104.9 | 0.038 | 0.929 |
| | Average/(kJ/mol) | 26.1 | | | 65.1 | | |

**Table S2** Most common reaction models for the thermal cracking of biomass tar model compounds.

| Symbol | Reaction mechanism | f(x) | G(x) |
|---|---|---|---|
| G1 | One-dimensional diffusion | $1/2x$ | $x^2$ |
| G2 | Two-dimensional diffusion (Valensi) | $[-\ln(1-x)]^{-1}$ | $x+(1-x)\ln(1-x)$ |
| G3 | Three-dimensional diffusion (Jander) | $1.5(1-x)2/3[1-(1-x)1/3]^{-1}$ | $[1-(1-x)1/3]^2$ |
| G4 | Three-dimensional diffusion (G-B) | $1.5[1-(1-x)1/3]^{-1}$ | $1-2x/3-(1-x)^{2/3}$ |
| G5 | Three-dimensional diffusion (A-J) | $1.5(1+x)2/3[(1+x)1/3-1]^{-1}$ | $[(1+x)1/3-1]^2$ |
| G6 | Chemical reaction (n=3) | $(1-x)^3$ | $[(1-x)^{-2}-1]/2$ |
| G7 | Chemical reaction (n=2) | $(1-x)^2$ | $(1-x)^{-1}-1$ |
| G8 | Chemical reaction (n=1) | $1-x$ | $-\ln(1-x)$ |
| G9 | Chemical reaction (n=0) | 1 | x |
| G10 | Nucleation and growth (n=2/3) | $1.5(1-x)\ [-\ln(1-x)]^{1/3}$ | $[-\ln(1-x)]^{2/3}$ |
| G11 | Nucleation and growth (n=1/2) | $2(1-x)\ [-\ln(1-x)]^{1/2}$ | $[-\ln(1-x)]^{1/2}$ |
| G12 | Nucleation and growth (n=1/3) | $3(1-x)\ [-\ln(1-x)]^{2/3}$ | $[-\ln(1-x)]^{1/3}$ |
| G13 | Nucleation and growth (n=1/4) | $4(1-x)\ [-\ln(1-x)]^{1/3}$ | $[-\ln(1-x)]^{1/4}$ |
| G14 | Autocatalytic reaction | $x\ (1-x)$ | $\ln[x/(1-x)]$ |
| G15 | Mampel power law (n=1/2) | $2x^{1/2}$ | $x^{1/2}$ |
| G16 | Mampel power law (n=1/3) | $3x^{2/3}$ | $x^{1/3}$ |
| G17 | Mampel power law (n=1/4) | $4x^{3/4}$ | $x^{1/4}$ |
| G18 | Contraction sphere | $3(1-x)^{2/3}$ | $1-(1-x)^{1/3}$ |
| G19 | Contraction cylinder | $2(1-x)^{1/2}$ | $1-(1-x)^{1/2}$ |

**Note:** A-J: Anti-Jander; G-B: Ginstling-Brounshtein.

**Table S3** Probable Reaction models and kinetic parameters for individual gas component during the thermal cracking of naphthalene.

| Gas | Temp | G(X) | G3 | G5 | G7 | G16 | G17 | Gas | Temp | G(X) | G2 | G3 | G6 | G16 | G17 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | Inter | -0.803 | -3.967 | -5.558 | -25.62 | -11.50 | | | Inter | -1.311 | -0.639 | -3.803 | -23.95 | -9.671 |
| | 700 °C | Slope | 0.052 | 0.251 | 0.383 | 1.652 | 0.762 | | 700 °C | Slope | 0.129 | 0.060 | 0.341 | 2.191 | 0.921 |
| | | lnK(t) | -2.943 | -1.379 | -0.959 | 0.502 | -0.271 | | | lnK(t) | -2.046 | -2.804 | -1.074 | 0.784 | -0.081 |
| | | $R^2$ | 0.969 | 0.823 | 0.994 | 0.872 | 0.958 | | | $R^2$ | 0.956 | 0.978 | 0.907 | 0.935 | 0.984 |
| | | Inter | -0.633 | -3.231 | -4.101 | -20.39 | -8.935 | | | Inter | -0.955 | -0.386 | -1.374 | -9.261 | -4.897 |
| | 750 °C | Slope | 0.048 | 0.236 | 0.341 | 1.527 | 0.698 | | 750 °C | Slope | 0.085 | 0.033 | 0.113 | 0.797 | 0.442 |
| | | lnK(t) | -3.019 | -1.443 | -1.073 | 0.423 | -0.358 | | | lnK(t) | -2.456 | -3.397 | -2.179 | -0.225 | -0.815 |
| | | $R^2$ | 0.954 | 0.978 | 0.924 | 0.988 | 0.975 | | | $R^2$ | 0.946 | 0.979 | 0.984 | 0.995 | 0.983 |
| | | Inter | -0.087 | -0.342 | -0.411 | -2.064 | -0.963 | | | Inter | -1.277 | -0.574 | -2.708 | -17.39 | - |
| | 800 °C | Slope | 0.033 | 0.108 | 0.258 | 0.775 | 0.438 | | 800 °C | Slope | 0.110 | 0.048 | 0.216 | 1.424 | 0.679 |
| $H_2$ | | lnK(t) | -3.410 | -2.225 | -1.353 | -0.254 | -0.823 | $CH_4$ | | lnK(t) | -2.199 | -3.035 | -1.532 | 0.353 | -0.386 |
| | | $R^2$ | 0.951 | 0.975 | 0.913 | 0.978 | 0.955 | | | $R^2$ | 0.970 | 0.990 | 0.927 | 0.961 | 0.995 |
| | | Inter | -0.125 | -0.975 | -0.423 | -5.508 | -1.776 | | | Inter | -0.713 | -0.243 | -0.581 | -4.563 | -2.923 |
| | 850 °C | Slope | 0.043 | 0.241 | 0.291 | 1.521 | 0.645 | | 850 °C | Slope | 0.044 | 0.014 | 0.033 | 0.285 | 0.191 |
| | | lnK(t) | -3.126 | -1.421 | -1.232 | 0.419 | -0.437 | | | lnK(t) | -3.117 | -4.219 | -3.389 | -1.252 | -1.653 |
| | | $R^2$ | 0.853 | 0.987 | 0.809 | 0.976 | 0.911 | | | $R^2$ | 0.927 | 0.958 | 0.994 | 0.966 | 0.936 |
| | | Inter | -0.202 | -1.769 | -0.926 | -10.43 | -3.291 | | | Inter | -0.270 | -0.112 | -0.386 | -2.390 | -1.196 |
| | 900 °C | Slope | 0.056 | 0.382 | 0.374 | 2.391 | 0.906 | | 900 °C | Slope | 0.063 | 0.023 | 0.069 | 0.512 | 0.302 |
| | | lnK(t) | -2.866 | -0.961 | -0.982 | 0.872 | -0.097 | | | lnK(t) | -2.754 | -3.745 | -2.664 | -0.669 | -1.194 |
| | | $R^2$ | 0.938 | 0.989 | 0.911 | 0.994 | 0.981 | | | $R^2$ | 0.890 | 0.938 | 0.991 | 0.970 | 0.933 |
| | **Ea** | **kJ/mol** | **0.3** | **33.9** | **4.9** | **11.8** | **3.6** | | **Ea** | **kJ/mol** | **39.7** | **51.7** | **84.2** | **75.4** | **58.6** |
| | Temp | G(X) | G3 | G6 | G7 | G16 | G17 | | Temp | Inter | G3 | G4 | G7 | G8 | G18 |
| | | Inter | -0.917 | -31.17 | -6.094 | -245.9 | -35.18 | | | Slope | -0.196 | 0.100 | -2.416 | -0.081 | 0.249 |
| | 700 °C | Slope | 0.110 | 3.222 | 0.771 | 25.23 | 3.834 | | 700 °C | lnK(t) | 0.053 | 0.012 | 0.470 | 0.189 | 0.035 |
| | | lnK(t) | -2.203 | 1.170 | -0.259 | 3.228 | 1.344 | | | $R^2$ | -2.927 | -4.386 | -0.754 | -1.663 | -3.350 |
| | | $R^2$ | 0.940 | 0.898 | 0.963 | 0.857 | 0.971 | | | Inter | 0.973 | 0.981 | 0.976 | 0.978 | 0.999 |
| | | Inter | -0.218 | -0.629 | -1.426 | -4.387 | -2.517 | | | Slope | 0.025 | 0.112 | 0.377 | 0.925 | 0.357 |
| | 750 °C | Slope | 0.020 | 0.054 | 0.162 | 0.418 | 0.258 | | 750 °C | lnK(t) | 0.029 | 0.009 | 0.208 | 0.091 | 0.021 |
| | | lnK(t) | -3.899 | -2.906 | -1.819 | -0.871 | -1.354 | | | $R^2$ | -3.511 | -4.660 | -1.566 | -2.386 | -3.820 |
| | | $R^2$ | 0.966 | 0.998 | 0.918 | 0.984 | 0.957 | | | Inter | 0.992 | 0.990 | 0.993 | 0.992 | 0.934 |
| | | Inter | -0.045 | -0.096 | -0.269 | -0.711 | -0.449 | | | Slope | 0.038 | 0.076 | 0.779 | 0.996 | 0.316 |
| $C_2H_4$ | 800 °C | Slope | 0.011 | 0.021 | 0.120 | 0.220 | 0.162 | $C_3H_8$ | 800 °C | lnK(t) | 0.019 | 0.008 | 0.117 | 0.057 | 0.016 |
| | | lnK(t) | -4.474 | -3.819 | -2.116 | -1.509 | -1.818 | | | $R^2$ | -3.954 | -4.793 | -2.141 | -2.854 | -4.079 |
| | | $R^2$ | 0.995 | 0.996 | 0.952 | 0.991 | 0.975 | | | Inter | 0.996 | 0.997 | 0.998 | 0.998 | 0.989 |
| | | Inter | -0.101 | -0.312 | -0.491 | -1.962 | -1.026 | | | Slope | -0.003 | 0.010 | 0.443 | 0.657 | 0.161 |
| | 850 °C | Slope | 0.020 | 0.053 | 0.161 | 0.413 | 0.256 | | 850 °C | lnK(t) | 0.007 | 0.005 | 0.053 | 0.033 | 0.011 |
| | | lnK(t) | -3.903 | -2.921 | -1.825 | -0.883 | -1.362 | | | $R^2$ | -4.8345 | -5.245 | -2.928 | -3.402 | -4.437 |
| | | $R^2$ | 0.996 | 0.990 | 0.975 | 0.999 | 0.993 | | | Inter | 0.999 | 0.999 | 0.999 | 0.999 | 0.994 |
| | | Inter | -0.151 | -0.428 | -0.954 | -2.96 | -1.701 | | | Slope | 0.251 | 0.181 | 1.994 | 1.630 | 0.520 |
| | 900 °C | Slope | 0.021 | 0.056 | 0.178 | 0.443 | 0.278 | | 900 °C | lnK(t) | 0.013 | 0.004 | 0.092 | 0.041 | 0.010 |
| | | lnK(t) | -3.833 | -2.871 | -1.722 | -0.813 | -1.277 | | | $R^2$ | -4.288 | -5.383 | -2.379 | -3.181 | -4.573 |
| | | $R^2$ | 0.996 | 0.979 | 0.979 | 0.997 | 0.996 | | | Inter | 0.992 | 0.999 | 0.999 | 0.999 | 0.993 |
| | **$E_a$** | **kJ/mol** | **66.1** | **162.5** | **49.1** | **162.1** | **105.3** | | **$E_a$** | **kJ/mol** | **27.2** | **0.4** | **17.8** | **6.9** | **1.1** |

**Table S4** Probable Reaction models and kinetic parameters for individual gas component during the thermal cracking of anthracene.

| Gas | Temp | G(X) | G3 | G5 | G7 | G9 | G18 | Gas | Temp | G(X) | G3 | G7 | G8 | G12 | G17 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | Inter | -0.091 | -0.037 | -0.848 | -0.256 | -0.227 | | | Inter | 0.039 | 0.673 | 0.998 | 0.487 | -3.527 |
| | 700 °C | Slope | 0.001 | 0.001 | 0.021 | 0.014 | 0.006 | | 700 °C | Slope | 0.027 | 0.179 | 0.082 | 0.189 | 0.828 |
| | | lnK(t) | -6.342 | -7.158 | -3.882 | -4.219 | -5.144 | | | lnK(t) | -3.593 | -1.719 | -2.490 | -1.665 | -0.188 |
| | | $R^2$ | 0.997 | 0.999 | 0.999 | 0.999 | 0.999 | | | $R^2$ | 0.973 | 0.981 | 0.974 | 0.978 | 0.999 |
| | | Inter | -0.162 | -0.017 | -0.698 | 0.198 | -0.105 | | | Inter | -0.144 | -0.494 | 0.427 | -0.792 | -8.178 |
| | 750 °C | Slope | 0.003 | 0.001 | 0.027 | 0.013 | 0.006 | | 750 °C | Slope | 0.039 | 0.252 | 0.118 | 0.269 | 1.134 |
| | | lnK(t) | -5.523 | -7.123 | -3.578 | -4.327 | -5.049 | | | lnK(t) | -3.242 | -1.374 | -2.130 | -1.310 | 0.126 |
| | | $R^2$ | 0.996 | 0.999 | 0.998 | 0.998 | 0.998 | | | $R^2$ | 0.994 | 0.990 | 0.993 | 0.992 | 0.934 |
| | | Inter | -0.001 | 0.052 | 0.238 | 0.983 | 0.336 | | | Inter | 0.136 | 1.381 | 1.291 | 1.193 | 1.088 |
| | 800 °C | Slope | 0.007 | 0.001 | 0.048 | 0.013 | 0.005 | | 800 °C | Slope | 0.013 | 0.083 | 0.041 | 0.091 | 0.294 |
| $H_2$ | | lnK(t) | -4.956 | -8.640 | -3.031 | -4.333 | -5.257 | $CH_4$ | | lnK(t) | -4.294 | -2.482 | -3.193 | -2.396 | -1.223 |
| | | $R^2$ | 0.996 | 0.995 | 0.996 | 0.996 | 0.996 | | | $R^2$ | 0.998 | 0.997 | 0.998 | 0.998 | 0.989 |
| | | Inter | -0.392 | 0.042 | -2.482 | 0.251 | 0.049 | | | Inter | 0.249 | 1.976 | 1.623 | 1.887 | 1.510 |
| | 850 °C | Slope | 0.013 | 0.001 | 0.090 | 0.024 | 0.009 | | 850 °C | Slope | 0.014 | 0.100 | 0.044 | 0.103 | 0.529 |
| | | lnK(t) | -4.332 | -8.039 | -2.399 | -3.707 | -4.637 | | | lnK(t) | -4.215 | -2.301 | -3.105 | -2.263 | -0.635 |
| | | $R^2$ | 0.998 | 0.982 | 0.999 | 0.998 | 0.996 | | | $R^2$ | 0.999 | 0.999 | 0.999 | 0.999 | 0.994 |
| | | Inter | -3.046 | -0.486 | -21.45 | -9.851 | -4.501 | | | Inter | 0.532 | 3.687 | 2.420 | 3.673 | 4.079 |
| | 900 °C | Slope | 0.049 | 0.008 | 0.351 | 0.168 | 0.074 | | 900 °C | Slope | 0.011 | 0.117 | 0.045 | 0.118 | 1.646 |
| | | lnK(t) | -3.009 | -4.824 | -1.044 | -1.781 | -2.596 | | | lnK(t) | -4.489 | -2.140 | -3.099 | -2.135 | 0.498 |
| | | $R^2$ | 0.971 | 0.924 | 0.991 | 0.958 | 0.971 | | | $R^2$ | 0.997 | 0.999 | 0.999 | 0.991 | 0.993 |
| | **Ea** | **kJ/mol** | **148.0** | **63.8** | **127.9** | **100.1** | **100.2** | | **Ea** | **kJ/mol** | **52.2** | **34.3** | **41.9** | **36.5** | **8.5** |
| | Temp | G(X) | G3 | G7 | G8 | G9 | G12 | | Temp | G(X) | G3 | G4 | G7 | G8 | G18 |
| | | Inter | -0.033 | -2.804 | -0.017 | 0.576 | -2.843 | | | Inter | -0.091 | -0.037 | -0.848 | -0.256 | -0.227 |
| | 700 °C | Slope | 0.016 | 0.188 | 0.071 | 0.040 | 0.189 | | 700 °C | Slope | 0.001 | 0.001 | 0.021 | 0.014 | 0.006 |
| | | lnK(t) | -4.090 | -1.667 | -2.643 | -3.216 | -1.663 | | | lnK(t) | -6.342 | -7.158 | -3.882 | -4.219 | -5.144 |
| | | $R^2$ | 0.996 | 0.984 | 0.988 | 0.989 | 0.984 | | | $R^2$ | 0.997 | 0.999 | 0.999 | 0.999 | 0.999 |
| | | Inter | -0.350 | -4.221 | -0.742 | 0.111 | -4.316 | | | Inter | -0.162 | -0.017 | -0.698 | 0.198 | -0.105 |
| | 750 °C | Slope | 0.022 | 0.202 | 0.080 | 0.046 | 0.204 | | 750 °C | Slope | 0.003 | 0.001 | 0.027 | 0.013 | 0.006 |
| | | lnK(t) | -3.812 | -1.595 | -2.518 | -3.065 | -1.586 | | | lnK(t) | -5.523 | -7.123 | -3.578 | -4.327 | -5.049 |
| | | $R^2$ | 0.998 | 0.988 | 0.992 | 0.994 | 0.989 | | | $R^2$ | 0.996 | 0.999 | 0.998 | 0.998 | 0.998 |
| | | Inter | -0.309 | -2.391 | -0.199 | 0.369 | -2.552 | | | Inter | -0.001 | 0.052 | 0.238 | 0.983 | 0.336 |
| $C_2H_4$ | 800 °C | Slope | 0.018 | 0.142 | 0.060 | 0.036 | 0.144 | $C_3H_8$ | 800 °C | Slope | 0.007 | 0.001 | 0.048 | 0.013 | 0.005 |
| | | lnK(t) | -3.971 | -1.953 | -2.808 | -3.321 | -1.931 | | | lnK(t) | -4.956 | -8.640 | -3.031 | -4.333 | -5.257 |
| | | $R^2$ | 0.999 | 0.997 | 0.998 | 0.999 | 0.997 | | | $R^2$ | 0.996 | 0.995 | 0.996 | 0.996 | 0.996 |
| | | Inter | -0.678 | -4.327 | -1.203 | -0.288 | -4.673 | | | Inter | -0.392 | 0.042 | -2.482 | 0.251 | 0.049 |
| | 850 °C | Slope | 0.025 | 0.173 | 0.077 | 0.047 | 0.179 | | 850 °C | Slope | 0.013 | 0.001 | 0.090 | 0.024 | 0.009 |
| | | lnK(t) | -3.672 | -1.754 | -2.558 | -3.044 | -1.715 | | | lnK(t) | -4.332 | -8.039 | -2.399 | -3.707 | -4.637 |
| | | $R^2$ | 0.995 | 0.989 | 0.993 | 0.995 | 0.991 | | | $R^2$ | 0.998 | 0.982 | 0.999 | 0.998 | 0.996 |
| | | Inter | 0.061 | 0.858 | 1.074 | 1.099 | 0.677 | | | Inter | -3.046 | -0.486 | -21.45 | -9.851 | -4.501 |
| | 900 °C | Slope | 0.007 | 0.045 | 0.021 | 0.013 | 0.048 | | 900 °C | Slope | 0.049 | 0.008 | 0.351 | 0.168 | 0.074 |
| | | lnK(t) | -4.939 | -3.092 | -3.848 | -4.311 | -3.033 | | | lnK(t) | -3.009 | -4.824 | -1.044 | -1.781 | -2.596 |
| | | $R^2$ | 0.998 | 0.997 | 0.998 | 0.998 | 0.998 | | | $R^2$ | 0.971 | 0.924 | 0.991 | 0.958 | 0.971 |
| | **Ea** | **kJ/mol** | **27.2** | **95.1** | **86.4** | **79.1** | **52.4** | | **$E_a$** | **kJ/mol** | **148.0** | **63.8** | **127.9** | **100.1** | **100.2** |