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// parameters.h for first order kinetics

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// Simulated experiments with first order kinetics, E=200 kJ mol⁻¹:

// Parameters: E=200kJ mol⁻¹, log10A=16 n=1.

const double ln\_10 =2.302585092994046; // to convert log10 A to ln A:

const double a[6]= {16.\*ln\_10, 0., 0., 0., 0., 0.};

const double b[3]= {200., 0., 0.};

const int nexper=6;

const double heating\_rate\_per\_min[nexper]=

{2.5, 5., 10., 15., 20., 40.};

// Format string to create file names

// %.1f formats heating rate

// %s formats an optional string " percent"

const char \*outfile\_fmt="E=200 lgA=16 heating rate=%.1f%s.txt";

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// parameters.h for TG approximation at heating rates

// 5, 10, 15 and 20 °C/min, linearly increasing E(α)

//

// Parameters for the curves in Fig. 2/A

// linear E(α), E(1)-E(0)=61.2 kJ mol⁻¹

// Model:

// dα/dt=exp[p(α)-E(α)/(RT)](1-α)

// x=2α-1 [-1≤x≤1]

// E(α)= 223.35713 +57.2x

// p(α)= 41.676932943 +11.805330285x -.141820821x² -.448214767x³

// -.547665259x⁴ +.510613902x⁵

const double a[6]={41.676932943, 11.805330285, -0.141820821, -0.448214767,

-0.547665259, 0.510613902};

const double b[3]= {223.35713, 57.2, 0.};

const int nexper=4;

const double heating\_rate\_per\_min[nexper]=

{5., 10., 15., 20.};

// Format string to create file names

// %.1f formats heating rate

// %s formats an optional string " percent"

const char \*outfile\_fmt="linear E, E(1)-E(0)=114 heating rate=%.1f%s.txt";

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// parameters.h for TG approximation at heating rates

// 2.5, 5, 10, 20 and 40 °C/min, linearly increasing E(α)

//

// Parameters for the curves in Fig. 2/B

// linear E(α), E(1)-E(0)=61.2 kJ mol⁻¹

// Model:

// dα/dt=exp[p(α)-E(α)/(RT)](1-α)

// x=2α-1 [-1≤x≤1]

// E(α)= 211.31871 +30.6x

// p(α)= 39.190251567 +6.353367853x -.082087159x² -.284291892x³ -.286423165x⁴ +

// +.311751601x⁵

const double a[6]={39.190251567, 6.353367853, -0.082087159, -0.284291892,

-0.286423165, 0.311751601};

const double b[3]= {211.31871, 30.6, 0.};

const int nexper=5;

const double heating\_rate\_per\_min[nexper]=

{2.5, 5., 10., 20., 40.};

// Format string to create file names

// %.1f formats heating rate

// %s formats an optional string " percent"

const char \*outfile\_fmt="linear E, E(1)-E(0)=61 heating rate=%.1f%s.txt";

/////////////////////////////////////////////////////////////////////////////////

// parameters.h for TG approximation at heating rates

// 5, 10, 15 and 20 °C/min, parabolic E(α)

//

// Parameters for the dashed E(α) curve in Fig. 1/B

// parabolic E(α), Emax-Emin=245.3 kJ mol⁻¹

// Model:

// dα/dt=exp[p(α)-E(α)/(RT)](1-α)

// x=2α-1

// E(α)= 177.77734 +78.5x +157.0x²

// p(α)= 32.223070251 +16.19636213x +32.116827133x² +.690895262x³

// -.075930046x⁴ -2.284201254x⁵

//

const double a[6]={32.223070251, 16.19636213, 32.116827133, 0.690895262,

-0.075930046, -2.284201254};

const double b[3]={177.77734,78.5,157.0};

const int nexper=4;

const double heating\_rate\_per\_min[nexper]={5., 10., 15., 20.};

// Format string to create file names

// %.1f formats heating rate

// %s formats an optional string " percent"

const char \*outfile\_fmt=

"parabolic E, Emax-Emin=245 heating rate=%.1f%s.txt";

/////////////////////////////////////////////////////////////////////////////////

// parameters.h for DTG approximation at heating rates

// 5, 10, 15 and 20 °C/min, linearly increasing E(α)

//

// Parameters for the curves in Fig. 4/A

// linear E(α), E(1)-E(0)=31.8 kJ mol⁻¹

// Model:

// dα/dt=exp[p(α)-E(α)/(RT)](1-α)

// x=2α-1 [-1≤x≤1]

// E(α)= 204.04473 +15.9x

// p(α)= 37.679813311 +3.273948575x -.075566238x² -.012339093x³

// -.099729566x⁴ +.061237711x⁵

const double a[6]={37.679813311, 3.273948575, -0.075566238, -0.012339093,

-0.099729566, 0.061237711};

const double b[3]= {204.04473, 15.9, 0.};

const int nexper=4;

const double heating\_rate\_per\_min[nexper]=

{5., 10., 15., 20.};

// Format string to create file names

// %.1f formats heating rate

// %s formats an optional string " percent"

const char \*outfile\_fmt="linear E, E(1)-E(0)=32 heating rate=%.1f%s.txt";

/////////////////////////////////////////////////////////////////////////////////

// parameters.h for DTG approximation at heating rates

// 2.5, 5, 10, 20 and 40 °C/min, linearly increasing E(α)

//

// Parameters for the curves in Fig. 4/B

// linear E(α), E(1)-E(0)=17 kJ mol⁻¹

// Model:

// dα/dt=exp[p(α)-E(α)/(RT)](1-α)

// x=2α-1 [-1≤x≤1]

// E(α)= 201.93157 +8.5x

// p(α)= 37.242485627 +1.755490645x -0.040069586x² -0.005244368x³ -0.055243622x⁴ +

// +0.030537805x⁵

const double a[6]={37.242485627, 1.755490645, -0.040069586, -0.005244368,

-0.055243622, 0.030537805};

const double b[3]={201.93157,8.5,0.};

const int nexper=5;

const double heating\_rate\_per\_min[nexper]=

{2.5, 5., 10., 20., 40.};

// Format string to create file names

// %.1f formats heating rate

// %s formats an optional string " percent"

const char \*outfile\_fmt="linear E, E(1)-E(0)=17 heating rate=%.1f%s.txt";

/////////////////////////////////////////////////////////////////////////////////

// parameters.h for DTG approximation at heating rates

// 5, 10, 15 and 20 °C/min, parabolic E(α)

//

// Parameters for the dashed E(α) curve in Fig. 3/B

// Parabolic E(α), E(1)-E(0)=45.6 kJ mol⁻¹

// Model:

// dα/dt=exp[p(α)-E(α)/(RT)](1-α)

// x=2α-1 [-1≤x≤1]

// E(α)= 199.55369 +14.6x +29.2x²

// p(α)= 36.748303663 +3.018648301x +5.943845265x² -.077744483x³

// +.037344246x⁴ -.228269076x⁵

const double a[6]={36.748303663, 3.018648301, 5.943845265, -0.077744483,

0.037344246, -0.228269076};

const double b[3]= {199.55369, 14.6, 29.2};

const int nexper=4;

const double heating\_rate\_per\_min[nexper]=

{5., 10., 15., 20.};

// Format string to create file names

// %.1f formats heating rate

// %s formats an optional string " percent"

const char \*outfile\_fmt="parabolic E, Emax-Emin=46 heating rate=%.1f%s.txt";