Standard Terminology Relating to
Hazard Potential of Chemicals[1]

1. Scope

1.1 This standard is a compilation of terminology used in the area of hazard potential of chemicals. Terms that are generally understood or adequately defined in other readily available sources are not included.

1.2 Although some of these definitions are general in nature, many must be used in the context of the standards in which they appear. The pertinent standard number is given in parentheses after the definition.

1.3 In the interest of common understanding and standardization, consistent word usage is encouraged to help eliminate the major barrier to effective technical communication.

2. Referenced Documents

2.1 *ASTM Standards:*[2]

E476 Test Method for Thermal Instability of Confined Condensed Phase Systems (Confinement Test) (Withdrawn 2008)[3]

E487 Test Method for Constant-Temperature Stability of Chemical Materials

E537 Test Method for The Thermal Stability of Chemicals by Differential Scanning Calorimetry

E582 Test Method for Minimum Ignition Energy and Quenching Distance in Gaseous Mixtures

E659 Test Method for Autoignition Temperature of Liquid Chemicals

E680 Test Method for Drop Weight Impact Sensitivity of Solid-Phase Hazardous Materials

E681 Test Method for Concentration Limits of Flammability of Chemicals (Vapors and Gases)

E698 Test Method for Arrhenius Kinetic Constants for Thermally Unstable Materials Using Differential Scanning Calorimetry and the Flynn/Wall/Ozawa Method

E771 Test Method for Spontaneous Heating Tendency of Materials (Withdrawn 2001)[3]

E918 Practice for Determining Limits of Flammability of Chemicals at Elevated Temperature and Pressure

E1226 Test Method for Explosibility of Dust Clouds

E1231 Practice for Calculation of Hazard Potential Figures-of-Merit for Thermally Unstable Materials

E1232 Test Method for Temperature Limit of Flammability of Chemicals

E1491 Test Method for Minimum Autoignition Temperature of Dust Clouds

E1515 Test Method for Minimum Explosible Concentration of Combustible Dusts

E1981 Guide for Assessing Thermal Stability of Materials by Methods of Accelerating Rate Calorimetry

E2012 Guide for the Preparation of a Binary Chemical Compatibility Chart

E2019 Test Method for Minimum Ignition Energy of a Dust Cloud in Air

E2021 Test Method for Hot-Surface Ignition Temperature of Dust Layers

E2046 Test Method for Reaction Induction Time by Thermal Analysis

3. Terminology

3.1 *Definitions:*

adiabatic calorimeter, *n*—an instrument capable of making calorimetric measurements while maintaining a minimal heat loss or gain between the sample and its environment, which is verifiable by the capability to continuously measure the temperature differential between the sample and its surroundings. **E1981**

adiabatic decomposition temperature rise, $(T)_d$, *n*—an estimation of the computed temperature which a specimen would attain if all of the enthalpy (heat) of decomposition reaction were to be absorbed by the sample itself. High values represent high hazard potential. **E1231**

anvil, *n*—the smooth, hardened surface upon which the test sample or cup containing the sample rests. **E680**

Arrhenius equation—k = $Ze^{-E/RT}$ where k is the specific reaction rate constant in reciprocal minutes for first order, Z is the pre-exponential factor in reciprocal minutes, E is the Arrhenius activation energy in J/mol, R is the gas constant, 8.32 J/mol K, and T is the temperature in kelvin.   **E698**

autoignition, *n*—the ignition of a material commonly in air as the result of heat liberation due to an exothermic oxidation reaction in the absence of an external ignition source such as a spark or flame.   **E659**

autoignition temperature, *n*—the minimum temperature at which autoignition occurs under the specified conditions of test.   **E659**

DISCUSSION—Autoignition temperature is also referred to as spontaneous ignition temperature, self-ignition temperature, autogenous ignition temperature, and by the acronyms AIT and SIT. AIT is the lowest temperature at which the substance will produce hot-flame ignition in air at atmospheric pressure without the aid of an external energy source such as spark or flame. It is the lowest temperature to which a combustible mixture must be raised, so that the rate of heat evolved by the exothermic oxidation reaction will over-balance the rate at which heat is lost to the surroundings and cause ignition.

compatibility, *adj*—the ability of materials to exist in contact without specified (usually hazardous) consequences under a defined scenario.   **E2012**

constant-temperature stability (CTS) value, *n*—the maximum temperature at which a chemical compound or mixture may be held for a 2-h period under the conditions of the test without exhibiting a measurable exothermic reaction.   **E487**

cool-flame, *n*—a faint, pale blue luminescence or flame occurring below the autoignition temperature (AIT).   **E659**

DISCUSSION—Cool-flames occur in rich vapor-air mixtures of most hydrocarbons and oxygenated hydrocarbons. They are the first part of the multistage ignition process.

critical half thickness, (a), *n*—an estimation of the half thickness of a sample in an *unstirred container*, in which the heat losses to the environment are less than the retained heat. This buildup of internal temperature leads to a thermal-runaway reaction.   **E1231**

critical temperature, (T_c), *n*—an estimation of the lowest temperature of an *unstirred container* at which the heat losses to the environment are less than the retained heat leading to a buildup of internal temperature. This temperature buildup leads to a thermal-runaway reaction.   **E1231**

DISCUSSION—This description assumes perfect heat removal at the reaction boundary. This condition is not met if the reaction takes place in an insulated container such as when several containers are stacked together or when a container is boxed for shipment. These figures-of-merit underestimate the hazard as a result of this underestimation of thermal conductivity.

deflagration index, (K_{St}), *n*—maximum *dP/dt* normalized to a 1.0 m³ volume. It is measured at the optimum dust concentration. K_{St} is defined according to the following cubic relationship:

$$K_{St} = (dP/dt)_{max}V^{1/3}$$

where:

P =   pressure, (bar),

t =   time, (s),
V =   volume, (m³), and
K_{St} =   (bar m/s).
   E1226

differential scanning calorimetry (DSC), *n*—a technique in which the difference in energy inputs into a substance and a reference material is measured as a function of temperature, while the substance and the reference material are subjected to a controlled temperature program.   **E698**

DISCUSSION—Two modes, power compensation differential scanning calorimetry (power compensation DSC) and heatflux differential scanning calorimetry (heatflux DSC), can be distinguished depending on the method of measurement used.

differential thermal analysis (DTA), *n*—a technique in which the temperature difference between a substance and reference material is measured as a function of temperature while the substance and the reference material are subjected to a controlled temperature program.   **E698**

(dP/dt)$_{ex}$, *n*—the maximum rate of pressure rise during the course of a single deflagration.   **E1226**

(dP/dt)$_{max}$, *n*—maximum value for the rate of pressure increase per unit time reached during the course of a deflagration for the optimum concentration of the dust tested. It is determined by a series of tests over a large range of concentrations. It is reported in bar/s.   **E1226**

drop weight, *n*—that weight which is raised to a selected height and released. This weight does not impact the sample directly; rather it strikes another stationary weight that is in contact with the sample.   **E680**

DTA (DSC) curve, *n*—a record of a thermal analysis where the temperature difference (ΔT) or the energy change (Δq) is plotted on the ordinate and temperature or time is plotted on the abscissa (see Figs. 3 and 4).   **E537**

dust concentration, *n*—the mass of dust divided by the internal volume of the test chamber.   **E1491**

extrapolated onset temperature, *n*—empirically, the temperature found by extrapolating the baseline (prior to the peak) and the leading side of the peak to their intersection (see Fig. 3).   **E537**

final temperature (T_{final}), *n*—the lowest temperature, corrected to a pressure of 101.3 kPa (760 mm Hg, 1013 mbar), at which application of an ignition source causes the vapors of the specimen to ignite under specified conditions of test.   **E1232**

flash point, *n*—the observed system temperature at the end of an exotherm, generally at the temperature where the self-heat rate of the reaction has decreased below the operator-defined slope sensitivity threshold. (1981)   **E1232**

general rate law—dC/dt = $k(1 - C)^n$ where C is fractional conversion, t is the time in minutes, and n is the reaction order.   **E698**

guide bushing, *n*—the steel bushing that surrounds, aligns, and holds the stationary intermediate weight in place.   **E680**

guide system, *n*—the rails, wires, and shaft that guide the drop weight during its fall. **E680**

hot-surface ignition temperature of a dust layer, *n*—lowest set temperature of the hot plate that causes ignition of the dust layer. **E2021**

H$_{50}$ value, *n*—a drop height with a 50 % probability of reaction, as determined experimentally by the Bruceton up-and-down method. **E680**

ideal adiabatic temperature rise (DTad), *n*—the temperature rise which would be observed in an exothermic reaction if all of the heat liberated were used to increase the temperature of only the sample. It is conveniently calculated as the product of the observed adiabatic temperature rise, DTobs, and the thermal inertia factor, f. **E1981**

ignition, *n*—the initiation of combustion. **E659**

ignition delay time, *n*—the time lapse between application of heat to a material and its ignition. It is the time in seconds between insertion of the sample into the flask and ignition. It is maximum at the minimum autoignition temperature and also referred to as ignition lag. **E659**

ignition delay time, t$_d$, *n*—experimental parameter defined as the time interval between the initiation of the dust dispersion procedure (the time at which the dispersion air starts to enter the chamber) in an experimental apparatus and the activation of the ignition source. The ignition delay time characterizes the turbulence level prevailing at ignition under the defined test conditions. **E1226**

ignition of a dust layer, *n*—initiation of self-heating or combustion in a material under test. **E2021**

ignition quenching distance, *n*—Maximum spacing between electrode flanges that will not permit spark ignition and flame propagation beyond the flanges, when tested under the specified test conditions. **E582**

ignition time, *n*—time between the start of heating and the point at which the maximum temperature or flaming combustion is reached. **E2021**

impact apparatus or machine, *n*—the total apparatus including the foundation parts, guide rails, electromagnet lift, winch, and tools. **E680**

impact tool, *n*—the drop weight, intermediate weight, and anvil. **E680**

lower limit of flammability or lower flammable limit (LFL), *n*—the minimum concentration of a combustible substance that is capable of propagating a flame through a homogeneous mixture of the combustible and a gaseous oxidizer under the specified conditions of test. **E681**

lower temperature limit of flammability, (LTL), *n*—the lowest temperature, corrected to a pressure of 101.3 kPa (760 mm Hg, 1013 mbar), at which application of an ignition source causes a homogeneous mixture of a gaseous oxidizer and vapors in equilibrium with a liquid (or solid) specimen

to ignite and propagate a flame away from the ignition source under the specified conditions of test. **E1232**

minimum autoignition temperature (MAIT), *n*—the minimum temperature at which a dust cloud will self ignite under the specified conditions of test. **E1515**

minimum explosible concentration (MEC), *n*—the minimum concentration of a combustible dust cloud that is capable of propagating a deflagration through a well dispersed mixture of the dust and air under the specified conditions of test **E1491**

minimum ignition energy, *n*—electrical energy discharged from a capacitor, which is just sufficient to effect ignition of the most ignitable mixture of a given fuel-mixture under specific test conditions. **E2019**

observed adiabatic temperature rise (DTobs), *n*—the observed temperature rise in the system during an exotherm; mathematically, it is equal to the temperature difference between the final temperature and the onset temperature of an exotherm. **E1981**

onset temperature, *n*—the temperature at which a deflection from the established baseline is first observed. **E537**

onset temperature (Tstart), *n*—the observed system temperature at the start of an exotherm where the self-heating rate first exceeds the operator-defined slope sensitivity threshold, usually 0.02°C/min; the onset temperature is not a fundamental property of a substance, but is apparatus-dependent, based upon the inherent sensitivity of the calorimetric system. (1981)

P$_{ex}$, *n*—the maximum explosion pressure (above the pressure in the vessel at the time of ignition) reached during the course of a single deflagration test. **E1226**

P$_{ignition}$, *n*—the absolute pressure at the time of ignition. **E1515**

P$_{ex,a}$, *n*—the maximum explosion pressure (absolute) reached during the course of a single deflagration test. **E1515**

ΔP$_{ignitor}$, *n*—the pressure rise in the chamber due to the ignitor by itself. **E1515**

P$_{max}$, *n*—the maximum pressure (above pressure in the vessel at the time of ignition) reached during the course of a deflagration for the optimum concentration of the dust tested. P_{max} is determined by a series of tests over a large range of concentrations. It is reported in bar. **E1226**

peak, *n*—that part of a DTA or DSC curve which is attributable to the occurrence of a single process. It is normally characterized by a deviation from the established base line, a maximum deflection, and a reestablishment of a base line not necessarily identical to that before the peak. **E698**

peak, *n*—that portion of a heating curve which is attributable to the occurrence of a single process. It is normally characterized by a deviation from the established baseline, a maximum deflection, and a reestablishment of a baseline not necessarily identical to that before the peak. **E537**

DISCUSSION—There will be instances when upon scanning in temperature an endotherm will be observed that is immediately followed by or is in conjunction with an exotherm. This type of competing reactions makes it difficult and at times impossible to locate the true peak and onset temperatures.

peak temperature, *n*—the temperature corresponding to the maximum deflection of the DTA or DSC curve.   **E537**

pressure ratio (PR), *n*—defined as PR= $(P_{ex,a}-\Delta P_{ignitor}/P_{ignition}.$ **E1515**

propagation of flame, *n*—the upward and outward movement of the flame front from the ignition source to the vessel walls, that is determined by visual observation.   **E918**

propagation of flames, *n*—as used in this practice, a combustion reaction that produces at least a 7 % rise of the initial absolute pressure:

$$\frac{P_2}{P_1} \geqq 1.07$$

E1232

DISCUSSION—This 7 % rise in pressure corresponds to 1 psia (0.007 MPa) per atmosphere of initial pressure.

reaction, *n*—any transformation of material accompanied by a change of enthalpy which may be endothermic or exothermic.   **E537**

reaction induction time (RIT) value, *n*—the time a chemical compound or mixture may be held under isothermal conditions until it exhibits a specified exothermic reaction. **E2046**

scenario, *n*—a detailed physical description of the process whereby a potential inadvertent combination of materials may occur.   **E2012**

self-heating, *adj*—any exothermic process which increases the temperature of the system by the self absorption of the liberated heat. (1981)

spark discharge, *n*—transient discrete electric discharge, which takes place between two conductors, which are at different potentials. The discharge bridges the gap between the conductors in the form of a single ionization channel.   **E2019**

spontaneous heating or self heating, *n*—an exothermic reaction of a material due to slow or incomplete reaction that results in a temperature rise above that of its surroundings.   **E771**

spontaneous heating temperature or self-heating temperature, *n*—the lowest temperature at which spontaneous or self heating occurs under the specified test conditions. This temperature refers to a much earlier stage of reaction than that associated with the autoignition temperature of the material.   **E771**

striking surface, *n*—the hardened, smooth, circular bottom surface of the intermediate tool that is in contact with the test sample.   **E680**

temperature rise, ΔT, *n*—the difference between T_{max} and the initial set temperature of the hot plate.   **E2021**

threshold temperature, *n*—temperature on the ΔT versus T curve where the slope changes in the direction indicating an exothermic reaction, that is, the sample is beginning to self-heat.   **E476**

time-to-maximum rate (TMR), *n*—the amount of time that is needed for a reaction to reach its maximum self-heating rate or pressure rate in a thermal runaway reaction, normally referenced from the time corresponding to the onset temperature, but may also be referenced from any time-temperature point to the time at which the maximum self-heating or pressure rate occurs. The experimentally observed TMR is normally divided by the thermal inertia factor (see 3.1.10) to obtain a more conservative assessment of TMR. (TMR divided by the thermal inertia factor is often referred to as the "f-corrected" TMR). (1981)   **E1231**

time-to-thermal-runaway, (t_c), *n*—an estimation of the time required for an exothermic reaction, in an adiabatic container, (that is, no heat gain or loss to the environment), to reach the point of thermal runaway.   **E1231**

T_{max}, *n*—maximum temperature measured during test. **E2021**

unconfined test, *n*—a test in which the test sample is placed directly upon the anvil with no lateral confinement.   **E680**

upper limit of flammability or upper flammable limit (UFL), *n*—the maximum concentration of a combustible substance that is capable of propagating a flame through a homogeneous mixture of the combustible and a gaseous oxidizer under the specified conditions of test.   **E681**