

PHD for Substance Reactions (OV-07 Logical Data Model Subject Area)
 System Architect
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 -Comment
 This diagram depicts the product hazard data that tracks the reactions associated with a substance, conditions that increase or decrease the likelihood that the reaction will occur, and the physical and chemical results when the reaction does occur.
 The ANSI standard for the Material Safety Data Sheet (MSDS) includes this information in Section 10, Stability and Reactivity.

Product Hazard Data for Substance Reactions

INGREDIENT
 Ingredient_Contained_Substance_Identifier . Substance_Identifier (FK)
 Ingredient_Greater_Substance_Identifier . Substance_Identifier (FK)
 Ingredient_Considered_De_Minimus_Indicator
 Ingredient_Considered_EPCRA_Hazardous_Indicator
 Ingredient_Considered_Impurity_Indicator
 Ingredient_Is_Stabilizer_Indicator
 Ingredient_Non_Numerical_Percent_Text
 Ingredient_Non_Numerical_Percent_Calculation_Text
 -Business Description
 A SUBSTANCE that is a direct constituent of another SUBSTANCE.
 For example, SUBSTANCE water is an INGREDIENT of SUBSTANCE 95% solution of Isopropyl Alcohol. SUBSTANCE Sodium Chloride is an INGREDIENT of SUBSTANCE saline solution. Elemental Tin is an INGREDIENT of pewter. Copper Oxide is an INGREDIENT of green paint.
 Note: A SUBSTANCE that is used in the manufacture of a second SUBSTANCE, but which does not retain its original molecular characteristics in the manufactured

SUBSTANCE
 Substance_Identifier . Material_Identifier (FK)
 Substance_State_Complexity_Type_Name
 Substance_Clarity_Name
 Substance_Color_Name
 Substance_Considered_Environmentally_Persistent_Indicator
 Substance_Inert_Indicator
 Substance_Gross_Structural_Type_Name
 Substance_Radioactive_Decay_Rate
 Substance_Radioactive_Decay_Rate_Unit_Of_Measure_Identifier . Unit_Of_Measure_Identifier (FK)
 Substance_Self_Reactive_Indicator
 Substance_Solid_Percent_By_Volume_Quantity
 Substance_Solid_Percent_By_Weight_Quantity
 Substance_Stable_Indicator
 Substance_Stability_Normal_Conditions_Text
 Substance_Volatile_Organic_Compound_Volume_Percent_Quantity
 Substance_Volatile_Organic_Compound_Volume_Non_Numeric_Quantity_Text
 Substance_Volatile_Organic_Compound_Weight_Percent_Quantity
 Substance_Volatile_Organic_Compound_Weight_Non_Numeric_Quantity_Text
 Substance_Water_N-Octanol_Partition_Coefficient_Quantity
 -Business Description
 A MATERIAL having no inherent limit in extent; therefore without size or shape. E.g., green paint, hydrochloric acid, dry ice, or Coke syrup.

CHEMICAL
 Chemical_Identifier . Substance_Identifier (FK)
 Chemical_Type_Name
 -Business Description
 A macroscopically homogenous SUBSTANCE that exists as such regardless of its physical state.
 Examples are gasoline, the secret ingredient in a popular soft drink, and depleted Uranium alloy.

SUBSTANCE-HAZARD
 Substance_Identifier (FK)
 Hazard_Identifier (FK)
 Substance_Hazard_Details_Text
 Substance_Hazard_Name
 Substance_Hazard_Primary_Danger_Indicator
 Substance_Hazard_Summary_Text
 -Business Description
 A HAZARD that has been determined to potentially result from the direct or indirect contact of persons, animals, plants, structures, property, equipment, or the environment to the relevant SUBSTANCE.

HAZARD
 Hazard_Identifier
 Hazard_Details_Text
 Hazard_Name
 Hazard_Summary_Text
 -Business Description
 A kind of negative effect potentially resulting from exposure of persons, animals, plants, structures, property, equipment, or the environment to a substance or its effects.

SUBSTANCE-REACTION-HAZARD
 Substance_Identifier (FK)
 Substance_Reaction_Distinguishing_Identifier (FK)
 Hazard_Identifier (FK)
 Substance_Reaction_Hazard_Details_Text
 Substance_Reaction_Hazard_Name
 Substance_Reaction_Hazard_Primary_Danger_Indicator
 Substance_Reaction_Hazard_Summary_Text
 -Business Description
 A HAZARD that has been determined to potentially result from the direct or indirect contact of persons, animals, plants, structures, property, equipment, or the environment to the relevant SUBSTANCE-REACTION.

SUBSTANCE-REACTION
 Substance_Identifier (FK)
 Substance_Reaction_Distinguishing_Identifier
 Substance_Reaction_Type_Name
 Substance_Reaction_Details_Text
 Substance_Reaction_Name
 Substance_Reaction_Summary_Text
 -Business Description
 A kind of chemical change or transformation whereby a SUBSTANCE decomposes, combines with one or more other SUBSTANCES, or interchanges constituents with one or more other SUBSTANCES.
 Examples are
 o the decomposition of benzyl peroxide into benzoic acid, benzene, carbon dioxide, and other substances,
 o the condensation of acetaldehyde, through a set of intermediate steps, ultimately into crotonaldehyde.

CONDITION-TO-AVOID-SUBSTANCE
 Condition_To_Avoid_Identifier (FK)
 Substance_Identifier (FK)
 -Business Description
 A CONDITION-TO-AVOID that applies to a SUBSTANCE.

CONDITION-TO-AVOID
 Condition_To_Avoid_Identifier
 Condition_To_Avoid_Details_Text
 Condition_To_Avoid_Name
 Condition_To_Avoid_Predefined_Indicator
 Condition_To_Avoid_Summary_Text
 -Business Description
 A kind of circumstance applicable to the use, storage, or transportation of substances that might result in a hazardous situation, and therefore should be avoided.

SUBSTANCE-REACTION-PRECONDITION
 Substance_Identifier (FK)
 Substance_Reaction_Distinguishing_Identifier (FK)
 Condition_To_Avoid_Identifier (FK)
 -Business Description
 A CONDITION-TO-AVOID that is necessary for the relevant SUBSTANCE-REACTION to happen.

STABILIZING-GROUP-SUBSTANCE
 Stabilizing_Group_Identifier (FK)
 Substance_Identifier (FK)
 -Business Description
 A SUBSTANCE that belongs to the relevant STABILIZING-GROUP.

STABILIZING-GROUP
 Stabilizing_Group_Identifier
 Stabilizing_Group_Details_Text
 Stabilizing_Group_Name
 Stabilizing_Group_Summary_Text
 -Business Description
 A set of one or more SUBSTANCES that can inhibit one or more SUBSTANCE-REACTIONS of another SUBSTANCE under normal circumstances.

SUBSTANCE-STABILIZATION
 Substance_Identifier (FK)
 Substance_Reaction_Distinguishing_Identifier (FK)
 Stabilizing_Group_Identifier (FK)
 Substance_Stabilization_Details_Text
 Substance_Stabilization_Summary_Text
 -Business Description
 A SUBSTANCE that has its SUBSTANCE-REACTIONS inhibited by the inclusion of one or members of the relevant STABILIZING-GROUP.

SUBSTANCE-CONDENSATION
 Substance_Identifier (FK)
 Substance_Reaction_Distinguishing_Identifier (FK)
 Substance_Condensation_Type_Name
 -Business Description
 A SUBSTANCE-REACTION during which at least one molecule of the SUBSTANCE interacts with at least one other molecule (perhaps of the same SUBSTANCE) through a series of addition and elimination steps that result in the generation of a large molecular weight SUBSTANCE and water (or, if not water, some other small molecular substance, such as ammonia or hydrogen sulfide).
 For example, the condensation of acetaldehyde, through a set of intermediate steps, ultimately into crotonaldehyde.

SUBSTANCE-REACTION-RESULTING-SUBSTANCE
 Substance_Reaction_Resulting_Substance_Original_Substance_Identifier . Substance_Identifier (FK)
 Substance_Reaction_Distinguishing_Identifier (FK)
 Substance_Reaction_Resulting_Substance_Identifier . Substance_Identifier (FK)
 -Business Description
 A SUBSTANCE that results from a SUBSTANCE-REACTION.

SUBSTANCE-INCOMPATIBLE-SUBSTANCE
 Substance_Incompatible_Substance_First_Substance_Identifier . Substance_Identifier (FK)
 Substance_Incompatible_Substance_Second_Substance_Identifier . Substance_Identifier (FK)
 Substance_Incompatible_Substance_Possible_Result_Details_Text
 Substance_Incompatible_Substance_Possible_Result_Summary_Text
 -Business Description
 A set of two SUBSTANCES that can react together to produce a hazardous situation.

REACTION-EFFECT
 Reaction_Effect_Identifier
 Reaction_Effect_Details_Text
 Reaction_Effect_Name
 Reaction_Effect_Predefined_Indicator
 Reaction_Effect_Summary_Text
 Reaction_Effect_Typically_Considered_Undesirable_Indicator
 -Business Description
 A condition, other than the generation of a new SUBSTANCE (or new ISOTOPE), that can result from a SUBSTANCE-REACTION (or RADIOISOTOPE decay).

SUBSTANCE-REACTION-EFFECT
 Substance_Identifier (FK)
 Substance_Reaction_Distinguishing_Identifier (FK)
 Reaction_Effect_Identifier (FK)
 -Business Description
 A REACTION-EFFECT that can result from a SUBSTANCE-REACTION.

