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Safe Operation Card (SOC)

Introduction: *The Safe Operation Card (SOC) is used as a tool to complete hazard assessment and planning for research activities as defined in The Dow Chemical Company R&D Management of Change Work Process.*

SAFE OPERATION CARD TEMPLATE

OWNER & CELL PHONE: _____ **APPROVED BY (TBD BY DEPT):** _____

OTHER PERSONNEL APPROVED TO RUN THIS REACTION OR OPERATION: _____

REVIEW PROCEDURE EVERY XX months. In-service date: _____ **REVIEW BY DATE:** _____

REACTION OR TYPE OF OPERATION (If synthesis, include: structures, names, and concentrations of chemicals to be used or made including reagents, catalysts, solvents, products, potential by-products if known), acceptable and "never exceed" ranges for temperatures & pressures, and comments on sampling and workups)

EMERGENCY SHUTDOWN PROCEDURES: Include location of plugs and devices, and label them.	
CHEMICAL EXPOSURE HAZARDS & RESPONSE: (Use worse case for each material used)	EYECONTACT: (example: may cause corneal irritation. Wash with water minimum of 15 minutes, contact emergency services (9-1-1)) SKIN CONTACT: INHALATION:
PERSONAL PROTECTIVE EQUIPMENT	EYE PROTECTION: (example: safety glasses for routine work, chemical goggles while pouring solvent into flask) BODY PROTECTION: REPSIRATORY PROTECTION:
SPILL CLEANUP/EQUIPMENT DECONTAMINATION RESPONSE: Are clean-up or decontamination supplies compatible and readily available?	
CHEMICAL, PHYSICAL OR MECHANICAL HAZARDS - Consider chemical compatibility, reactivity, flammability, explosion potential, toxicity. Can your equipment handle rapid evolution of volumes of gas? Are you inerting equipment if you are operating at temperatures above the flash point of a solvent? - Consider Pressure, Temperature, Corrosivity, Electrical Hazards, Cylinder Storage/Use	

HAZARD EVALUATION TOOLS

Hazard Level Assessment for Synthesis or Operation:
Classified as "HIGH" if any of the following is YES:

High Toxicity / Low exposure limits (Use MSDS for information)	Yes / No
High/Moderate Hazard Reaction performed ≤ 2 times – See Tables 3 & 5 below.	Yes / No
HOT chemistry (> 400 J/g mixture if <1L, > 200 J/g mixture if 1-5L, > 100 J/g mixture if >5 L). The rate of reaction could increase to a thermal explosion if any of the control systems fail (cooling, agitation, addition controllers, etc)	Yes / No
Using flammable gases, liquids, or solids (FP <38C, LFL <10 vol% in air, AIT < 200C)	Yes / No
High Hazard Reaction or Functional Group (See Table 6)	Yes / No
Chemicals are: air/moisture sensitive, pyrophoric, combustible dusts, impact sensitive, polymerizable, water reactive, corrosive, require an inhibitor, heat sensitive, or may react explosively?	Yes / No
Extreme Reaction Temperature (>150C or < -30C)?	Yes / No
High Temperature Feed (>50 C)?	Yes / No
High Pressure Reaction (>10 bar) or Feed (>2 bar)?	Yes / No
OVERALL Hazard Level Assessment – Circle High if any of the above are "Yes"	**High / Not High**

Reactive ChemicalsChecklists

MSDS (Material Safety Data Sheets) Reviewed	Yes / No
You have received training on this SOC card	Yes / No
Do reactants or products contain functional groups or atom groupings that confer explosive properties to the molecule (R1, R2, R3, R6, R8, R9)? Complete Reactive Chemicals Checklist for Explosibility Potential.	Yes / No
Are you working with R4, R5, R16, R19 or R44 chemicals? Complete Reactive Chemicals Checklist for R4, 5, 16, 19, 44	Yes / No

Overall Hazard Mitigation / Risk Reduction Assessment

OVERALL Hazard Level Assessment: If "HIGH", VERIFY that the planned activity has been reevaluated using the high level review checklist and additional reviews were held as appropriate to identify additional protective measures – Circle Yes or No.	Yes / No / NA
Reactive Chemicals Checklist (R1, R2, R3, R6, R8, R9) - I have put controls in place to manage or mitigate the hazards to reduce the risk of an unplanned event	Yes / No / NA
Reactive Chemicals Checklist (R4, R5, R16, R19, R44) - I have put controls in place to manage or mitigate the hazards to reduce the risk of an unplanned event	Yes / No / NA
When prompted to STOP, I have reevaluated my planned activity and sought additional review(s) to to identify additional protective measures and mitigate hazards before proceeding.	Yes / No / NA

Reactive Chemicals Checklist - Explosivity Potential

Specific Hazard (with European Union R-Phrase)	"N" is Prompt to STOP and Control/Mitigate Hazard	Y	N	NA
(R1) – Explosive when dry **(R2) – Risk of explosion by shock, friction, fire or other sources of ignition** **(R3) – Extreme risk of explosion by shock, friction, fire or other sources of ignition** **(R6) – Explosive with or without contact with air** **(R8) – Contact with combustible material may cause fire** **(R9) – Explosive when mixed with combustible substances** (e.g. Peroxides, Diazo Compounds, Nitro, Nitrite, Nitrate, Chlorates, Perchlorates or Bromates) Circle which apply. If any do apply, use next column and assess if controls are in place to manage or mitigate the hazards.	**(R1, 2, 3, 6, 8, 9) If "yes" or "I'm not sure" to ANY of these check boxes, then STOP! Reevaluate planned activity and modify as appropriate to mitigate the hazard before proceeding.** ☐ Are there any credible hazardous scenarios with handling the material neat or dry such that all the potential energy can be released? ☐ When handling heat sensitive or shock sensitive materials, I could accidently initiate an explosion from heat or frictional force. ☐ The pressure I could generate from an unintended event can exceed the burst pressure of my equipment, instrument, or reaction vessel. ☐ I could isolate neat, energetic intermediates or products with these properties during my reaction, work-up, or subsequent reaction steps. ☐ I could injure myself or cause structural damage if an explosion occurs. ☐ I could accidentally mix incompatible chemicals, absorbents, or contact incompatible metals during storage, use, and disposal.	☐	☐	☐

Reactive Chemicals Checklist - R4, R5, R16, R19, R44

Specific Hazard (with European Union R-Phrase) "N" is Prompt to STOP and Control/Mitigate Hazard	Y	N	NA	Specific Hazard (with European Union R-Phrase) "N" is Prompt to STOP and Control/Mitigate Hazard	Y	N	NA
(R4) - Forms very sensitive explosive metallic compounds - For example, metal azides (M-N3), metal hydrazines (M-N=N), metal acetylides (M-C≡C) , metal fulminates (M-C=N-O or C=N-O-M) Ag (silver metal) + HNO3 (nitric acid) + ROH (alcohol) -> Ag(+)R≡N-O (silver fulminate) or AgNO3 (silver nitrate) + ROH (alcohol) -> Ag(+)R≡N-O (silver fulminate) **- but you can you prevent accidental or intended mixing of samples, reagents, standards, or wastes that may cause the formation of explosive, highly unsaturated R4 metal compounds. Check Y=Yes or N=No. NA if R4 does not apply.** *If "No", STOP! Reevaluate planned activity and modify as appropriate to mitigate the hazard before proceeding.*	☐	☐	☐	**(R16) - Explosive when mixed with oxidizing substance -** **- but you can you mitigate this hazard.** Check Y=Yes or N=No. NA if R16 does not apply. Hazard mitigation is YES if any of these inherently safe practices apply: (Indicate which will be used) ☐ No credible scenarios with accidental or intended mixing with oxidizers during storage, use, and disposal. ☐ Equipment, instrument, or vessel will contain or safely relieve, not rupture, from worst-case pressures or pressure rates. ☐ Segregate reactive wastes ☐ Always use dilute vs. neat energetic materials *If "No", STOP! Reevaluate planned activity and modify as appropriate to mitigate the hazard before proceeding.*	☐	☐	☐
	Y	N	NA		Y	N	NA
(R5) - Heating may cause an explosion - Examples of R5 materials with this property include: hydroxylamine, perchloric acid, hydrogen peroxide, etc. **- but you can you store, use, and dispose of the R5 material in a manner to prevent it from releasing all its energy at once. Check Y=Yes or N=No. NA if R5 does not apply.** This is YES if any of these inherently safe practices apply: (Indicate which will be used) ☐ Temperature monitoring and control during storage and use to avoid fast rates of reaction or decomposition that may cause reaction vessels or sample containers to rupture. ☐ Segregate from incompatible chemicals or materials of construction which, upon mixing, could result in heat or pressure generation. ☐ Excess solvent (providing ebullient cooling) ☐ Using dilute vs. neat energetic materials *If "No", STOP! Reevaluate planned activity and modify as appropriate to mitigate the hazard before proceeding.*	☐	☐	☐	**(R19) - May form explosive peroxides -** Check Y=Yes or N=No. NA if R19 does not apply. **- but there is a low risk because the bottle been opened < 3 months, the chemical has been stored under an inert atmosphere, or it has shown negative in a peroxide test** *If "No", STOP! Reevaluate planned activity and modify as appropriate to mitigate the hazard before proceeding.*	☐	☐	☐
				- but you can you PREVENT forming or concentrating peroxides as a reaction by-product or in distillation overheads *If "No", STOP! Reevaluate planned activity and modify as appropriate to mitigate the hazard before proceeding.*	☐	☐	☐
				(R44) - Risk of explosion if heated under confinement - Examples: propane cylinders, mixed compressed gases, etc. **- but you can PREVENT heating liquid or compressed gases under confinement.** Check Y=Yes or N=No. NA if R44 does not apply. *If "No", STOP! Reevaluate planned activity and modify as appropriate to mitigate the hazard before proceeding.*	☐	☐	☐

TABLE 3. Reactions Having a High Hazard Potential

Reference Guide for Hazard Level Assessment [1] - No Need to Post with SOC Card.

Reaction	Example of concern
Curtis Rearrangements	Use of acyl azides, nitrous acid or hydrazine.
Decarboxylation	Removal of -COOH with CO_2 evolution. Possible over-pressure hazard.
Diazotizations	Especially if followed by reduction to the hydrazine ($SnCl_2$ reaction); replacement with a –OH, or to replace -NH_2 with -H
Displacements	Uses oxalyl chloride to displace -OH. (CO_2, CO, HCl generated)
Epoxidations	Epoxides are high energy strained rings
Esterification	When using oxalyl chloride
Friedel Crafts ($AlCl_3$)	Friedel Crafts reactions and their quenches due to use of $AlCl_3$, BCl_3, H_2SO_4, HF.
Grignard reactions	Reactions require an activation period and are highly exothermic.
Hydrolysis	Hydrolysis of a cyano to an amide oxidatively using H_2O_2
Metallations	Uses *n*-BuLi, *t*-BuLi, LDA, NaHMDS
Nitrations	Uses nitric acid and strong acids like sulfuric or triflic acid (trifluoromethylsulfonic acid). Nitrations are very exothermic. Potential exists for thermal runaway, initiating violent decompositions and explosions.
Oxidations	Use of Jones reagent [$K_2Cr_2O_7/H_2SO_4$], O_3, H_2O_2, $KMnO_4$ (with large exotherms), peroxo acids, cleavage using sodium periodate
Peptide formations	Use of HOBT (Hydroxybenzotriazole hydrate).
Quenches	When PCl_5 or $POCl_3$ have been used in a previous step and water is the quench
Reductions	Any nitro compound or high energy functional group reduction. Reductions using $LiAlH_4$, Fe or Zn powder with HCl or acetic acid, hydrazine in caustic; hydrogenations by generating H_2 in-situ using hydrazine, $NaBH_4$ in CH_3OH or C_6H_{12}
Sulfonation	Sulfonation of an amine to form sulfonamide

[1] Leggett, D.; "Chemical Reactivity Assessments in R&D", *Journal of Hazardous Materials*, **115(1–3),** 63-70 (2004). A Collection of Papers Presented at the Annual Symposium of the Mary Kay O'Connor Process Safety Centre, Texas A and M University, College Station, TX, United States, 28-29 October, 2003

TABLE 5. Reactions Having a Moderate Hazard Potential

Reference Guide for Hazard Level Assessment [1] - No Need to Post with SOC Card.

Reaction	Examples of concern
Acylations	Use of acetic anhydride or acid chloride acylations of amines.
Additions	Additions of alkyl metals to ketones or aldehydes, cyano groups, carboxylic acids or esters, or any other functionalities.
Alkylations	Alkyl halide or amine (aromatic or aliphatic) used with a phenol.
BOC protections-deprotections	BOC (*t*-butoxycarbonyl) used to protect/deprotect amines. Unreacted BOC anhydride in waste streams can liberate CO_2 and isobutylene.
Condensations	C–C bond or C–N bond formation with elimination of small molecules.
Cross coupling reactions	These reactions involve the use of a metal to mediate a C–C bond formation, usually a Pd(0) species (Pd(triphenyl-phosphine)$_4$; Suzuki coupling; zincate coupling by transmetalating a Grignard or a lithium species with zinc chloride.
Dealkylation	Demethylation of methoxy group using HBr or HCl to generate methyl bromide or methyl chloride. BBr_3 and $BC1_3$ used at low temperatures.
Displacement	Displacement of -OH with -Cl using PCl5; reactions are heated, the distilled PCl5 is difficult to quench due to the delayed water reaction. Use of LiCl in NMP to displace a triflate (CF3SO3−).
Esterification	Using oxalyl chloride and acid followed by alcohol addition. Reaction liberates CO and HCl–pressure hazard. Also by using acid and SOCl2 and then adding the alcohol.
Ether formations	Ethers formed via Williamson synthesis by alkylating with alkylhalide.
Halogenations	Reactions of alkyl or aryl groups with halogens such as Br2 Cl2 or I2.
Hydrolysis	Reaction of a cyano with Lewis acid (e.g. BF3). See other categories for hydrolysis/quench reactions.
Peptide formations	Coupling of an amine with an acid using EDC, EEDQ (N-ethoxycarbonyl-2-ethoxy-1,2-dihydroquinoline), or alkyl-chloroformate mediated peptide coupling, or N-hydroxy succinamide.
Reductions	Use of triethylsilane, NaBH4 (except with methanol), tri-acetoxyborohydride, B2H6 generated in-situ via BF3/NaBH4. Birch reductions with Na or K is category. Reductions using H2 and Pd, Pt, Raney Ni, Ru, Ir.
Sulfonation	Use of SO2Cl2 with an alcohol (plus base) to form a mesylate or tosylate. Use of triflic anhydride to form a triflate

[1] Leggett, D.; "Chemical Reactivity Assessments in R&D", *Journal of Hazardous Materials*, **115(1–3),** 63-70 (2004). A Collection of Papers Presented at the Annual Symposium of the Mary Kay O'Connor Process Safety Centre, Texas A and M University, College Station, TX, United States, 28-29 October, 2003.

TABLE 6. Atomic Groupings in a Molecule Indicating Potentially Explosive Characteristics

Reference Guide for Hazard Level Assessment [1] No Need to Post with SOC Card.

Table 6. Atom groupings that indicate or enhance molecular instability

Atom grouping with molecule	Example of functional group	
	Structure	Name
C· C and C· N triple bonds & their metal salts	· C· C· ; · C· N	Acetylenic; cyano
Adjacent N· O atoms many combinations	C· NO_2; C· O· N· O	Aryl, alkyl nitro; alkyl nitrite
Adjacent and consecutive N atom pairs, triplets and higher	· C· N· N; · N· N· N	Diazo; azide
Adjacent O· O pairs	· C· O· O· H; C· O· O· C	Peroxyacids; peroxyesters, peroxides
Adjacent C atoms bridged by O or N and many ring combinations of 4 or less atoms		Epoxides, azetidine
O· X atomic pairs	· O· X; · ClO_3	Hypohalites; chlorates
Many N· metal atomic pairs	· N· M	N· metal salts

[1] Leggett, D.; "Chemical Reactivity Assessments in R&D", *Journal of Hazardous Materials*, **115(1–3),** 63-70 (2004). A Collection of Papers Presented at the Annual Symposium of the Mary Kay O'Connor Process Safety Centre, Texas A and M University, College Station, TX, United States, 28-29 October, 2003.

NOTE: This list of atomic groupings is not exhaustive. For more information about specific explosive reactivity hazards indexed by chemical or class of chemicals, see Bretherick's Handbook of Reactive Chemical Hazards, Volumes 1-2 (7th Edition) Edited by: Urben, Peter G. © 2007 Elsevier