VERTEX
THE SCIENCE *of* POSSIBILITY

USING THE O.R.E.O.S. TOOL FOR EXPLOSIVE HAZARD IDENTIFICATION

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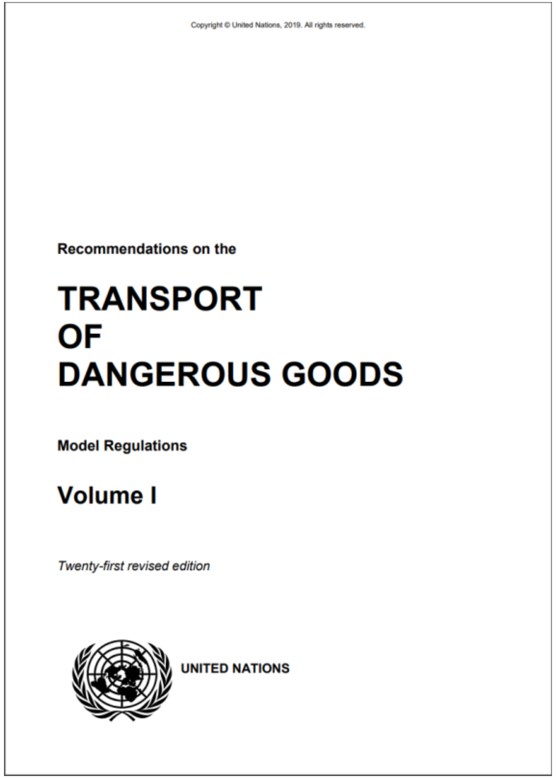
PRESENTED AT THE SPRING MEETING OF THE PURDUE PROCESS SAFETY AND ASSURANCE CENTER

MAY 10, 2022

DEFINITION OF EXPLOSIVE SUBSTANCE

"Explosive substance" is defined in 2.1.1.3 (a) of U.N. Model Regulations:

"Explosive substance is a solid or liquid substance (or a mixture of substances) which is in itself capable by chemical reaction of producing gas at such a temperature and pressure and at such a speed as to cause damage to the surroundings. Pyrotechnic substances are included even when they do not evolve gases"



Recommendations on the

TRANSPORT
OF
DANGEROUS GOODS

Model Regulations

Volume I

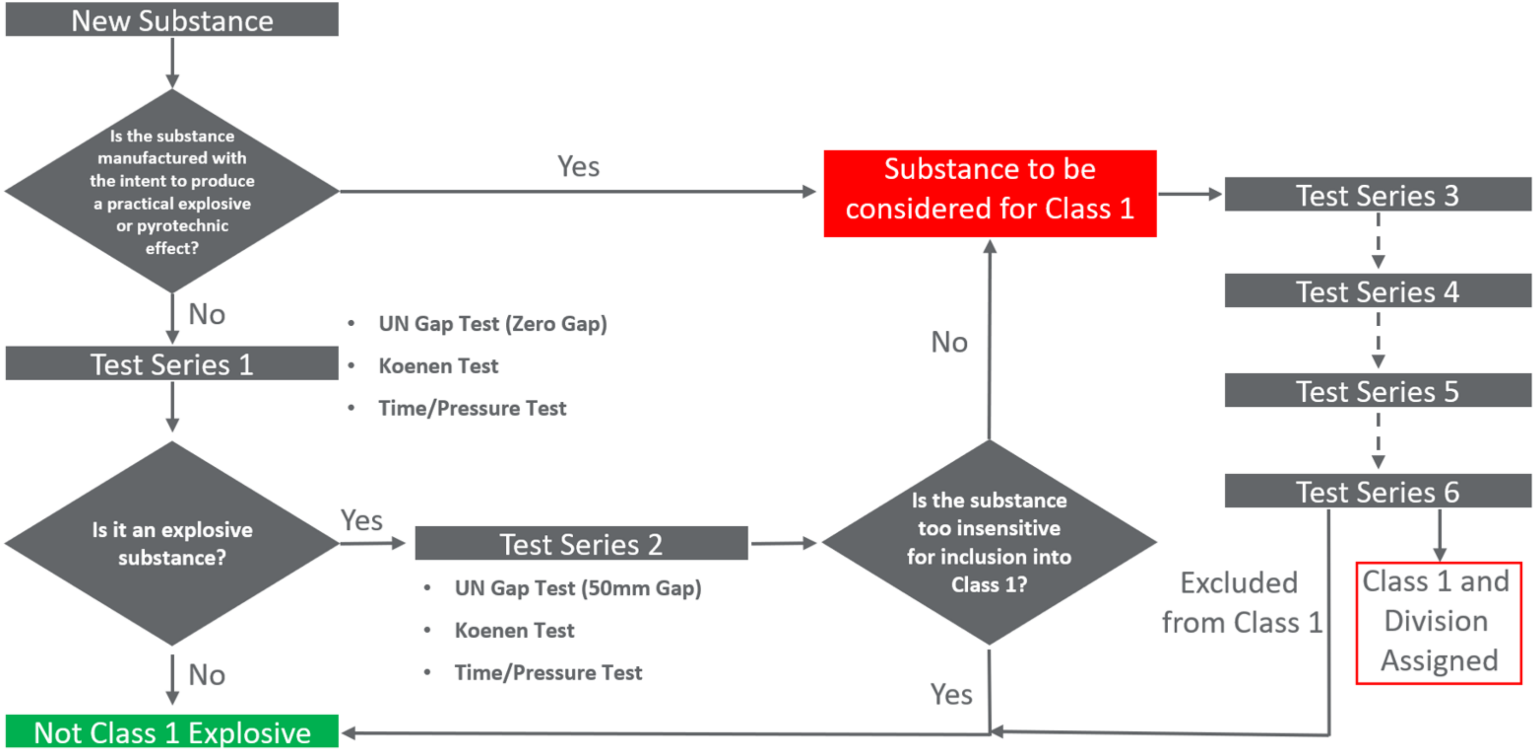
Twenty-first revised edition

UNITED NATIONS

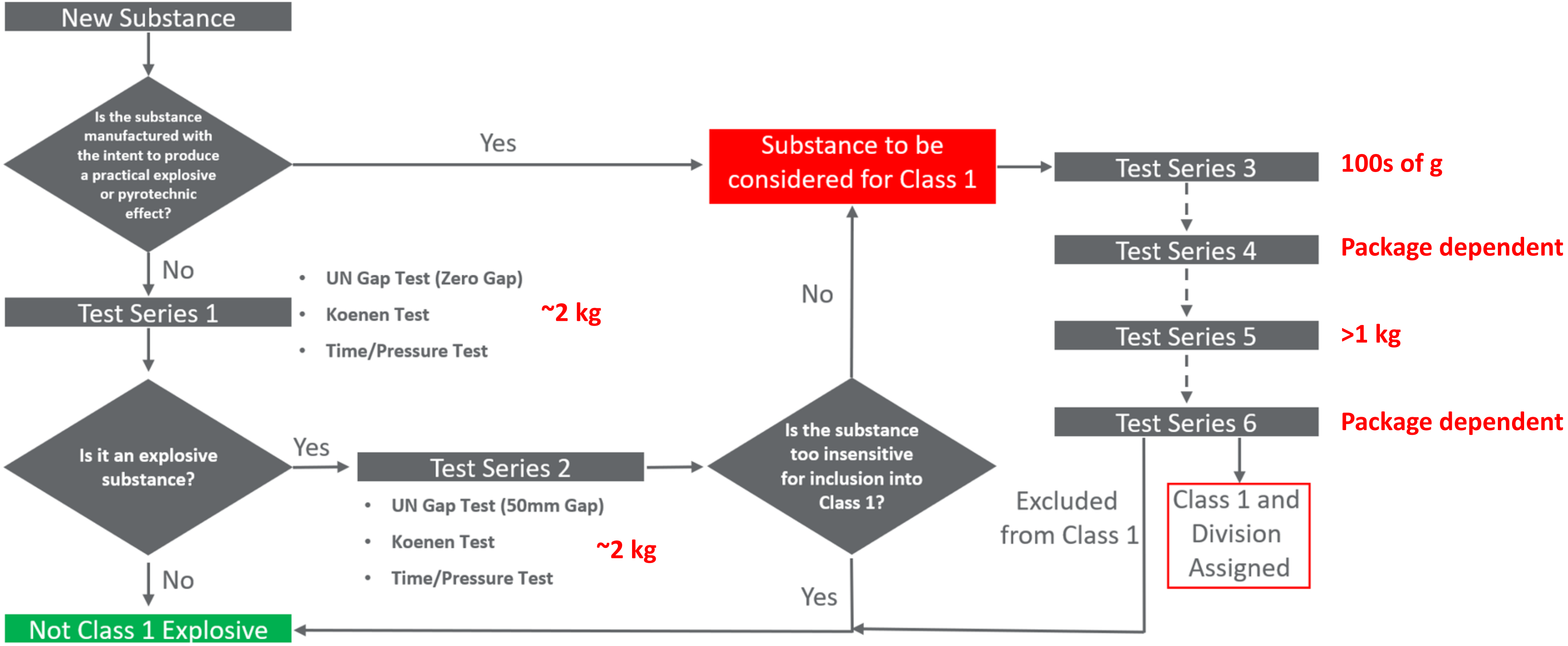
https://www.unece.org/trans/danger/publi/unrec/rev21/21files_e.html

CLASSIFYING EXPLOSIVE SUBSTANCES PER U.N. MODEL REGULATIONS (UNMR)

CLASSIFYING EXPLOSIVE SUBSTANCES



CLASSIFYING EXPLOSIVE SUBSTANCES

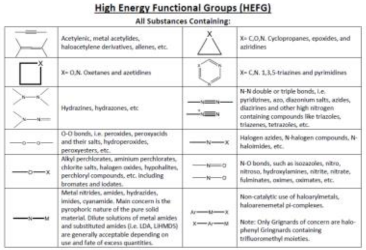


DSC WORKFLOW AT VERTEX PHARMACEUTICALS

OUR WORKFLOW

OUR WORKFLOW

Identify HEFGs



High Energy Functional Groups (HEFG)

All Substances Containing:

	Acetylenic, metal acetylides, haloacetylene derivatives, allenes, etc.		X= C,O,N. Cyclopropanes, epoxides, and aziridines
	X= O,N. Oxetanes and azetidines		X= C,N. 1,3,5-triazines and pyrimidines
	Hydrazines, hydrazones, etc		N-N double or triple bonds, i.e. pyridizines, azo, diazonium salts, azides, diazirines and other high nitrogen containing compounds like triazoles, triazenes, tetrazoles, etc.
	O-O bonds, i.e. peroxides, peroxyacids and their salts, hydroperoxides, peroxyesters, etc.		Halogen azides, N-halogen compounds, N-haloimides, etc.
	Alkyl perchlorates, aminium perchlorates, chlorite salts, halogen oxides, hypohalites, perchloryl compounds, etc. including bromates and iodates.		N-O bonds, such as isozazoles, nitro, nitroso, hydroxylamines, nitrite, nitrate, fulminates, oximes, oximates, etc.
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OUR WORKFLOW

Identify HEFGs

Perform DSC Testing

High Energy Functional Groups (HEFG)

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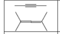
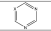
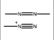
	Acetylenic, metal acetylides, haloacetylene derivatives, allenes, etc.		X= C,O,N. Cyclopropanes, epoxides, and aziridines
	X= O,N. Oxetanes and azetidines		X= C,N. 1,3,5-triazines and pyrimidines
	Hydrazines, hydrazones, etc		N-N double or triple bonds, i.e. pyridizines, azo, diazonium salts, azides, diazirines and other high nitrogen containing compounds like triazoles, triazenes, tetrazoles, etc.
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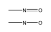
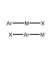
	Alkyl perchlorates, aminium perchlorates, chlorite salts, halogen oxides, hypohalites, perchloryl compounds, etc. including bromates and iodates.		N-O bonds, such as isozazoles, nitro, nitroso, hydroxylamines, nitrite, nitrate, fulminates, oximes, oximates, etc.
	Metal nitrides, amides, hydrazides, imides, cyanamide. Main concern is the pyrophoric nature of the pure solid material. Dilute solutions of metal amides and substituted amides (i.e. LDA, LiHMDS) are generally acceptable depending on use and fate of excess quantities.		Non-catalytic use of haloarylmetals, haloarenemetal pi-complexes. Note: Only Grignards of concern are halo-phenyl Gringnards containing trifluoromethyl moieties.

OUR WORKFLOW

Identify HEFGs → Perform DSC Testing → Apply Yoshida Correlations

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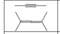
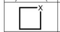
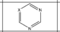
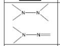
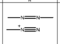
	Acetylenic, metal acetylides, haloacetylene derivatives, allenes, etc.		X= C,O,N. Cyclopropanes, epoxides, and aziridines
	X= O,N. Oxetanes and azetidines		X= C,N. 1,3,5-triazines and pyrimidines
	Hydrazines, hydrazones, etc		N-N double or triple bonds, i.e. pyridizines, azo, diazonium salts, azides, diazirines and other high nitrogen containing compounds like triazoles, triazenes, tetrazoles, etc.
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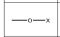
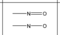
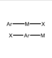
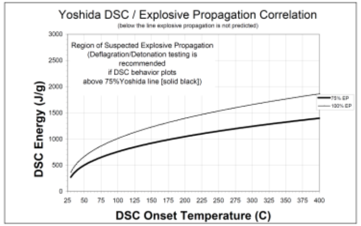
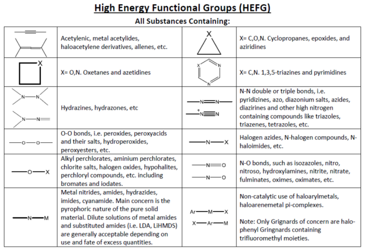
	Alkyl perchlorates, aminium perchlorates, chlorite salts, halogen oxides, hypohalites, perchloryl compounds, etc. including bromates and iodates.		N-O bonds, such as isozazoles, nitro, nitroso, hydroxylamines, nitrite, nitrate, fulminates, oximes, oximates, etc.
	Metal nitrides, amides, hydrazides, imides, cyanamide. Main concern is the pyrophoric nature of the pure solid material. Dilute solutions of metal amides and substituted amides (i.e. LDA, LiHMDS) are generally acceptable depending on use and fate of excess quantities.		Non-catalytic use of haloarylmetals, haloarenemetal pi-complexes. Note: Only Grignards of concern are halo-phenyl Gringnards containing trifluoromethyl moieties.



OUR WORKFLOW

Identify HEFGs → Perform DSC Testing → Apply Yoshida Correlations → Explosive? / Shock Sensitive?



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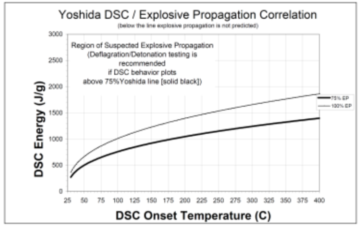

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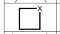
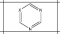
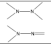
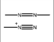
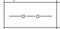
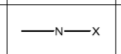
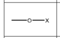
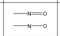
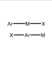
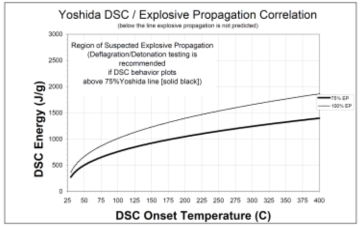
	X= O,N. Oxetanes and azetidines		X= C,N. 1,3,5-triazines and pyrimidines
	Hydrazines, hydrazones, etc		N-N double or triple bonds, i.e. pyridizines, azo, diazonium salts, azides, diazirines and other high nitrogen containing compounds like triazoles, triazenes, tetrazoles, etc.
	O-O bonds, i.e. peroxides, peroxyacids and their salts, hydroperoxides, peroxyesters, etc.		Halogen azides, N-halogen compounds, N-haloimides, etc.
	Alkyl perchlorates, aminium perchlorates, chlorite salts, halogen oxides, hypohalites, perchloryl compounds, etc. including bromates and iodates.		N-O bonds, such as isozazoles, nitro, nitroso, hydroxylamines, nitrite, nitrate, fulminates, oximes, oximates, etc.
	Metal nitrides, amides, hydrazides, imides, cyanamide. Main concern is the pyrophoric nature of the pure solid material. Dilute solutions of metal amides and substituted amides (i.e. LDA, LiHMDS) are generally acceptable depending on use and fate of excess quantities.		Non-catalytic use of haloarylmetals, haloarenemetal pi-complexes. Note: Only Grignards of concern are halo-phenyl Gringnards containing trifluoromethyl moieties.



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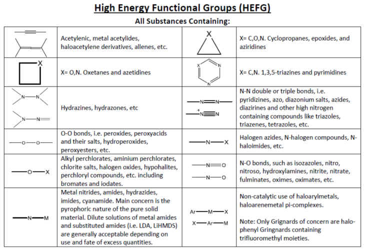
Identify HEFGs → Perform DSC Testing → Apply Yoshida Correlations → Explosive? → ???????

Apply Yoshida Correlations → Shock Sensitive? → Impact Testing



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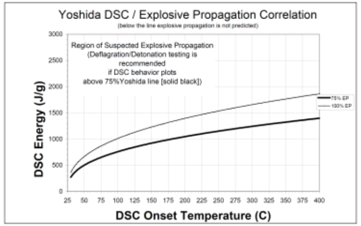

EXPLOSIVITY SCREENING METHODOLOGIES

SCREENING METHODOLOGIES

- HEFG List
- Yoshida Correlation (Explosive Propagation)
- Oxygen Balance calculation
- “Rule of Six”
- Explosive Functional Group (ExFG) list

HEFG LIST

- A high-energy functional group (HEFG) is any functional group that is known to contribute to the exothermic decomposition of a molecule
- Compounds containing one or more HEFGs may be unsafe at any temperature
- The more HEFGs a compound has, the more exothermic its decomposition and the less stable

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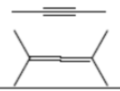
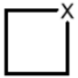
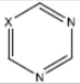
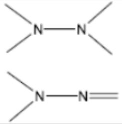
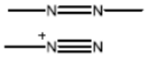
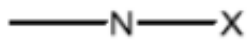
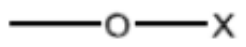
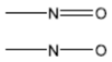
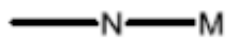
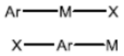
	Acetylenic, metal acetylides, haloacetylene derivatives, allenes, etc.		X= C,O,N. Cyclopropanes, epoxides, and aziridines
	X= O,N. Oxetanes and azetidines		X= C,N. 1,3,5-triazines and pyrimidines
	Hydrazines, hydrazones, etc		N-N double or triple bonds, i.e. pyridizines, azo, diazonium salts, azides, diazirines and other high nitrogen containing compounds like triazoles, triazenes, tetrazoles, etc.
	O-O bonds, i.e. peroxides, peroxyacids and their salts, hydroperoxides, peroxyesters, etc.		Halogen azides, N-halogen compounds, N-haloimides, etc.
	Alkyl perchlorates, aminium perchlorates, chlorite salts, halogen oxides, hypohalites, perchloryl compounds, etc. including bromates and iodates.		N-O bonds, such as isozazoles, nitro, nitroso, hydroxylamines, nitrite, nitrate, fulminates, oximes, oximates, etc.
	Metal nitrides, amides, hydrazides, imides, cyanamide. Main concern is the pyrophoric nature of the pure solid material. Dilute solutions of metal amides and substituted amides (i.e. LDA, LiHMDS) are generally acceptable depending on use and fate of excess quantities.		Non-catalytic use of haloarylmetals, haloarenemetal pi-complexes. Note: Only Grignards of concern are halo-phenyl Gringnards containing trifluoromethyl moieties.

THE YOSHIDA CORRELATIONS

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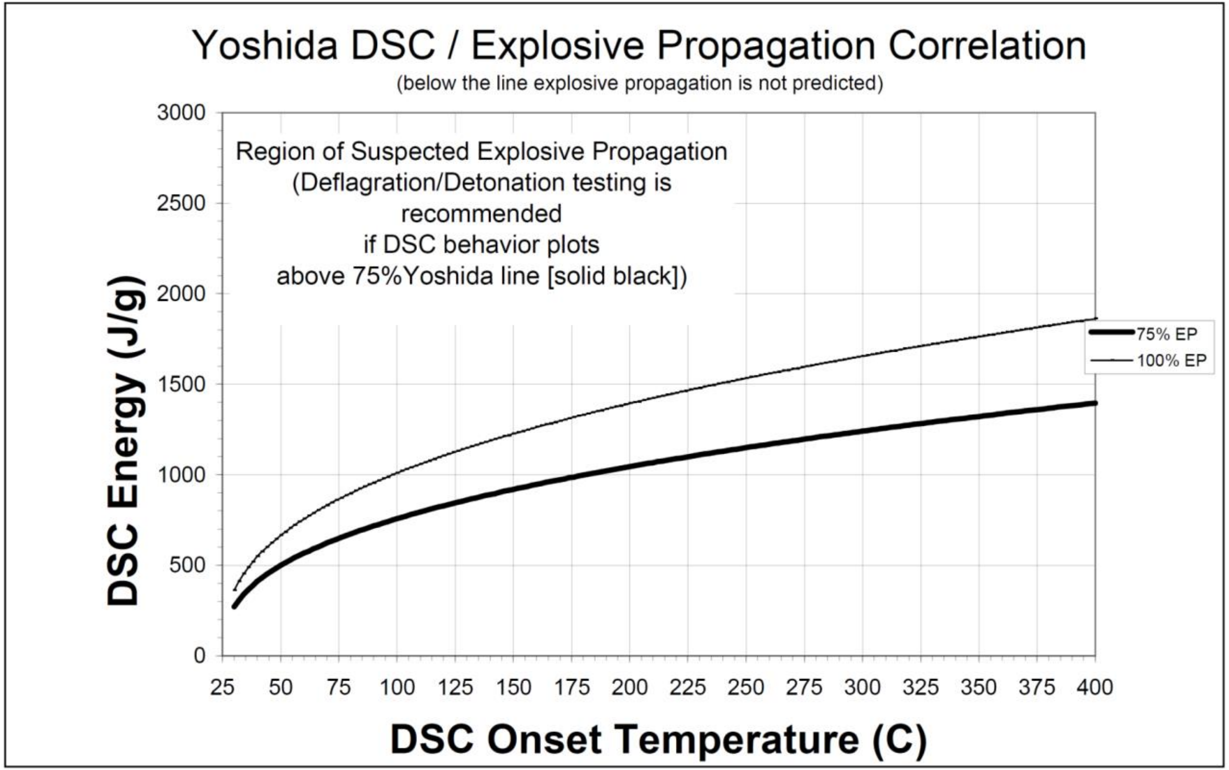
- Mathematical equation used to predict explosive properties as a function of DSC onset temperature and the energy associated with any exothermic decompositions

$$EP = \log(Q_{DSC}) - 0.38[\log(T_{DSC} - 25)] - 1.67$$

Q_{DSC} is the energy of the exotherm in cal/g, and T_{DSC} is the onset temperature of the exotherm in °C

YOSHIDA CORRELATION FOR EXPLOSIVE PROPAGATION



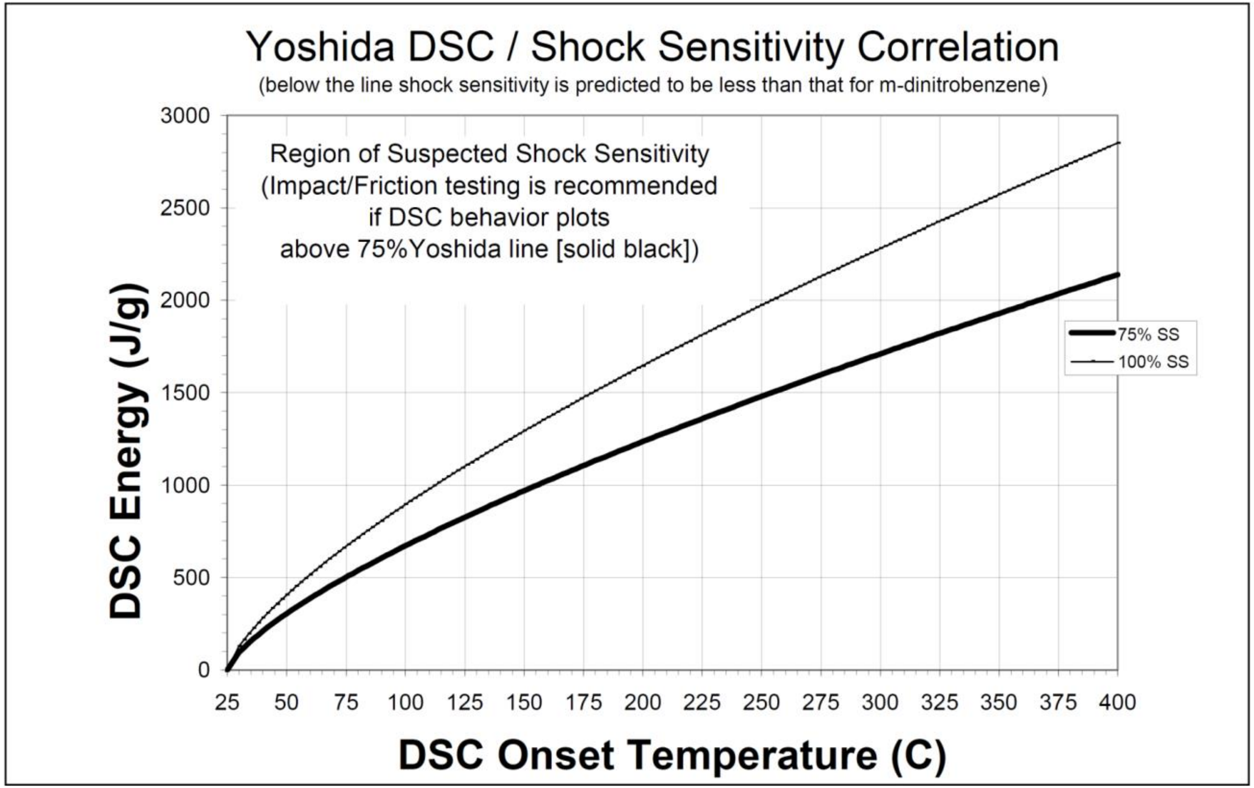
YOSHIDA CORRELATION FOR SHOCK SENSITIVITY

- Mathematical equation used to predict explosive properties as a function of DSC onset temperature and the energy associated with any exothermic decompositions

$$EP = \log(Q_{DSC}) - 0.72[\log(T_{DSC} - 25)] - 0.98$$

Q_{DSC} is the energy of the exotherm in cal/g, and T_{DSC} is the onset temperature of the exotherm in °C

YOSHIDA CORRELATION FOR SHOCK SENSITIVITY



EXPLOSIVE FUNCTIONAL GROUPS

EXFG LIST

- An explosive functional group (ExFG) is a functional group that can give a molecule explosive properties
- Every ExFG is also an HEFG but not all HEFGs are ExFGs
- The more ExFGs a compound has, the more likely it is to be classified as an explosive material

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- The more ExFGs a compound has, the more likely it is to be classified as an explosive material

Structural Feature	Examples
C – C Unsaturation	Acetylene, acetylides, 1,2-dienes (allenes)
C-Metal, N-Metal	Grignard reagents, organo-lithium species
Contiguous nitrogen atoms	Azides, aliphatic azo compounds, diazonium salts, hydrazines, sulfonyl hydrazides
Contiguous oxygen atoms	Peroxides, ozonides
N-O	Nitro, nitroso, nitrates, hydroxylamines, N-oxides, 1,2-oxazoles
N-halogen, O-halogen	Chloramines, fluoroamines, chlorates, perchlorates, iodosyl compounds

https://pubs.acs.org/doi/pdf/10.1021/acs.oprd.0c00467

RULE OF SIX

RULE OF SIX

Rule of 6

- Introduced by Peer in 1998
- Originally applied to azides but has since been applied to other materials containing explosive functional groups
- The “Rule of Six” states: **If a substance presents at least six atoms of carbon (or other atoms of approximately the same size) per energetic functionality (ExFG), this should render the molecule relatively safe to handle**

Peer, M. *Spec. Chem*. **1998**, *18*, 256 - 263.

IDENTIFYING CHEMICAL HAZARDS – RULE OF SIX

If a substance presents at least six atoms of carbon (or other atoms of approximately the same size) per energetic functionality (ExFG), this should render the molecule relatively safe to handle

Rule of Six Pass or Fail?

IDENTIFYING CHEMICAL HAZARDS – RULE OF SIX

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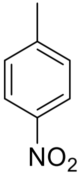
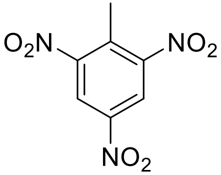
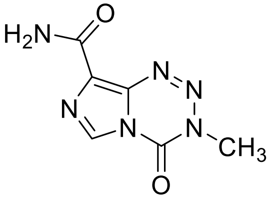
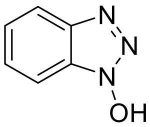
Rule of Six Pass or Fail?







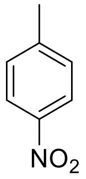
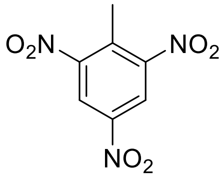
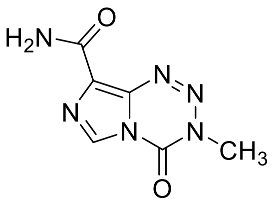
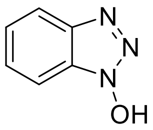


Rule of Six:	Pass	Fail	Pass	
Explosive?	No	Yes	Yes	Yes
Safe to Handle?	Yes	No	Yes	No

IDENTIFYING CHEMICAL HAZARDS – RULE OF SIX

If a substance presents at least six atoms of carbon (or other atoms of approximately the same size) per energetic functionality (ExFG), this should render the molecule relatively safe to handle

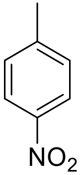
Rule of Six Pass or Fail?

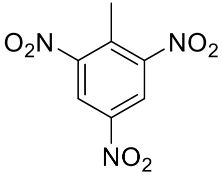
				
Rule of Six:	Pass	Fail	Pass	Depends
Explosive?	No	Yes	Yes	Yes
Safe to Handle?	Yes	No	Yes	No

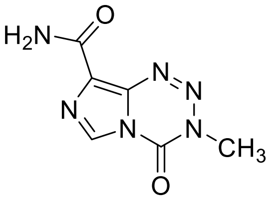
IDENTIFYING CHEMICAL HAZARDS – RULE OF SIX

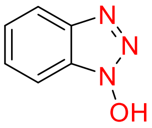
If a substance presents at least six atoms of carbon (or other atoms of approximately the same size) per energetic functionality (ExFG), this should render the molecule relatively safe to handle

Rule of Six Pass or Fail?







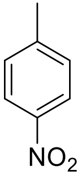


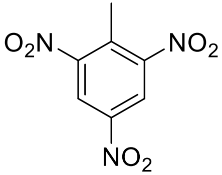
Rule of Six:	Pass	Fail	Pass	Depends
Explosive?	No	Yes	Yes	Yes
Safe to Handle?	Yes	No	Yes	No

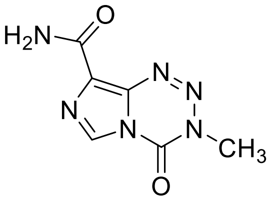
IDENTIFYING CHEMICAL HAZARDS – RULE OF SIX

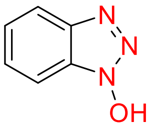
If a substance presents at least six atoms of carbon (or other atoms of approximately the same size) per energetic functionality (ExFG), this should render the molecule relatively safe to handle

Rule of Six Pass or Fail?









Rule of Six:	Pass	Fail	Pass	Depends 1 ExFG = Pass; 2 ExFG = Fail
Explosive?	No	Yes	Yes	Yes
Safe to Handle?	Yes	No	Yes	No

OXYGEN BALANCE

OXYGEN BALANCE CALCULATION

Oxygen Balance: For an organic compound with a molecular formula of $C_XH_YO_Z$ and molecular weight (MW), the OB can be obtained by the following equation:

Shanley, E. S.; Melhem, G. A. *Process Saf. Prog.* **1995**, *14*, 29– 31

OXYGEN BALANCE CALCULATION

<u>Oxygen Balance:</u> For an organic compound with a molecular formula of $C_XH_YO_Z$ and molecular weight (MW), the OB can be obtained by the following equation:

$$Oxygen\ Balance = \frac{\left[-1600\left(2X+\frac{Y}{2}-Z\right)\right]}{MW}$$

Shanley, E. S.; Melhem, G. A. *Process Saf. Prog.* **1995**, *14*, 29– 31

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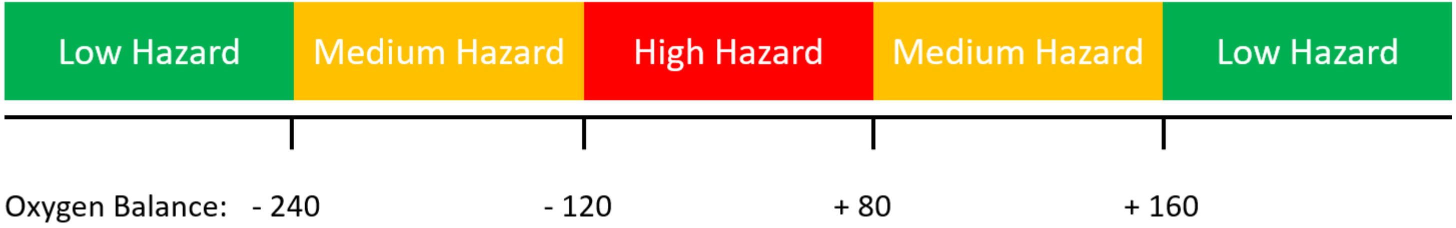


Shanley, E. S.; Melhem, G. A. *Process Saf. Prog.* **1995**, *14*, 29– 31

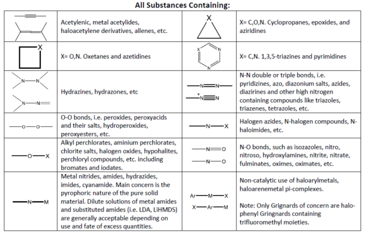
OXYGEN BALANCE CALCULATION

Compound	Oxygen Balance	Oxygen Balance Hazard Rank	Observed Hazard Rank
Hydrogen Peroxide	47	High	Medium-High
Water	0	High	None
Oxalic Acid	-18	High	None
Hydrazoic acid	-19	High	High
Acetyl peroxide	-95	High	High
Diazomethane	-114	High	High
t-Butyl Peroxide	-252	Low	High
Ethylene	-286	Low	Medium
Acetylene	-308	Low	High

OUR WORKFLOW

Identify HEFGs — Perform DSC Testing — Apply Yoshida Correlations

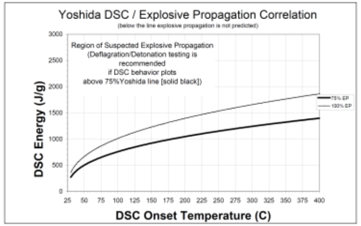
- Explosive? — ???????
- Shock Sensitive? — Impact Testing



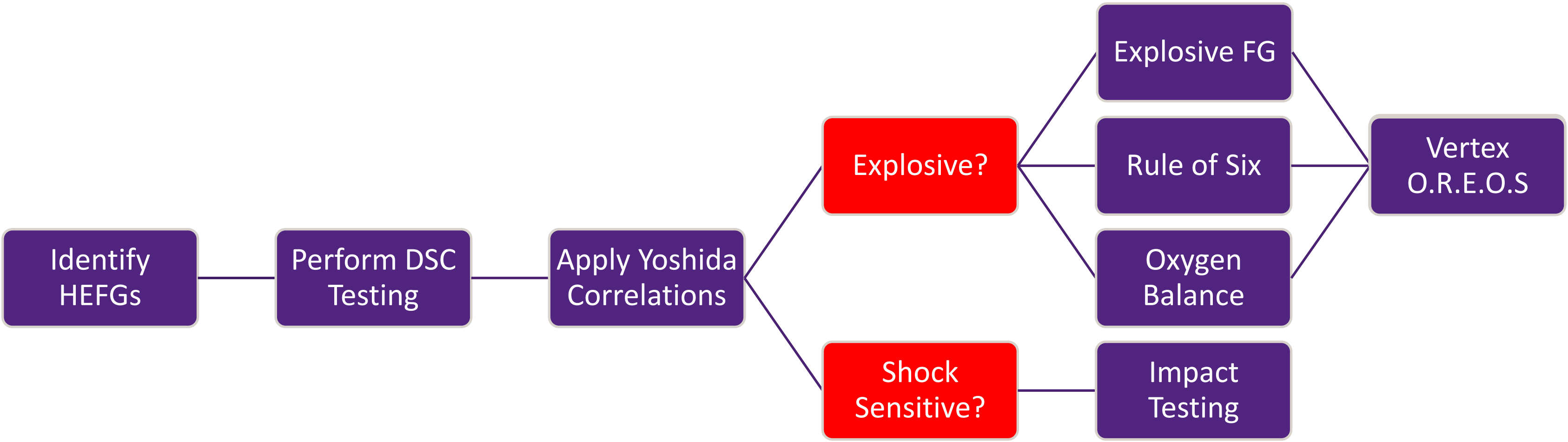
High Energy Functional Groups (HEFG)

All Substances Containing:

	Acetylenic, metal acetylides, haloacetylene derivatives, allenes, etc.		X= C,O,N. Cyclopropanes, epoxides, and aziridines
	X= O,N. Oxetanes and azetidines		X= C,N. 1,3,5-triazines and pyrimidines
	Hydrazines, hydrazones, etc		N-N double or triple bonds, i.e. pyridizines, azo, diazonium salts, azides, diazirines and other high nitrogen containing compounds like triazoles, triazenes, tetrazoles, etc.
	O-O bonds, i.e. peroxides, peroxyacids and their salts, hydroperoxides, peroxyesters, etc.		Halogen azides, N-halogen compounds, N-haloimides, etc.
	Alkyl perchlorates, aminium perchlorates, chlorite salts, halogen oxides, hypohalites, perchloryl compounds, etc. including bromates and iodates.		N-O bonds, such as isozazoles, nitro, nitroso, hydroxylamines, nitrite, nitrate, fulminates, oximes, oximates, etc.
	Metal nitrides, amides, hydrazides, imides, cyanamide. Main concern is the pyrophoric nature of the pure solid material. Dilute solutions of metal amides and substituted amides (i.e. LDA, LiHMDS) are generally acceptable depending on use and fate of excess quantities.		Non-catalytic use of haloarylmetals, haloarenemetal pi-complexes. Note: Only Grignards of concern are halo-phenyl Gringnards containing trifluoromethyl moieties.



OUR WORKFLOW



THE VERTEX O.R.E.O.S. TOOL

O.R.E.O.S. TOOL

- Combine <u>o</u>xygen balance calculation, the "<u>R</u>ule of 6" and the <u>e</u>xplosive functional group list together and combined with a material's <u>o</u>nset temperature of decomposition and the proposed <u>s</u>cale
- O.R.E.O.S. is effective at combining the five variables into a single hazard category
- This tool aims to identify materials early in Discovery that could pose additional risk (rapid pressure events), before any large-scale chemistry is planned
- This tool is also fully customizable for any organization to align with the internal Environmental Health and Safety and/or Laboratory Safety guidance for handling energetic materials since both the "Onset Temperature" and "Scale" variables can be modified
- Only requires a 3-5mg sample for DSC analysis

O.R.E.O.S. TOOL

	Points			
	1	2	4	8
Oxygen Balance Hazard		Low	Med	High
Rule of 6 calculation		Pass		Fail
Explosive Functional Group?	No			Yes
Onset temperature	>300	200-300	125-200	<125
Scale	1mg to 5g	5g to 100g	101g to 500g	>500g
O.R.E.O.S. Total:				
		Low Hazard	Medium Hazard	High Hazard
	Points:	7 to 17	18 to 27	28 to 40

APPLYING O.R.E.O.S. TOOL

	Points			
	1	2	4	8
Oxygen Balance Hazard		Low	Med	High
Rule of 6 calculation		Pass		Fail
Explosive Functional Group?	No			Yes
Onset temperature	>300	200-300	125-200	<125
Scale	1mg to 5g	5g to 100g	101g to 500g	>500g
O.R.E.O.S. Total:				
		Low Hazard	Medium Hazard	High Hazard
	Points:	7 to 17	18 to 27	28 to 40

Low Hazard	• Proceed using internal guidance on handling energetic compounds.
	• ARC testing ***recommended***. ***-or-*** • Quantitative small-scale explosivity screening is ***recommended***

Quantitative small-scale explosivity screening: mini-autoclave or ARC with high-speed pressure transducer

https://pubs.acs.org/doi/10.1021/acs.oprd.0c00467

APPLYING O.R.E.O.S. TOOL

	Points			
	1	2	4	8
Oxygen Balance Hazard		Low	Med	High
Rule of 6 calculation		Pass		Fail
Explosive Functional Group?	No			Yes
Onset temperature	>300	200-300	125-200	<125
Scale	1mg to 5g	5g to 100g	101g to 500g	>500g
O.R.E.O.S. Total:				
		Low Hazard	Medium Hazard	High Hazard
	Points:	7 to 17	18 to 27	28 to 40

Medium Hazard	• Proceed using internal guidance on handling energetic compounds.
	• ARC testing is ***required***. ***-or-*** • Quantitative small-scale explosivity screening is ***required***
	• Select Test Series 1 is ***recommended*** based on ARC testing, likely failure modes and available material (Koenen Test, Time/Pressure Test, and/or U.N. Gap)

Quantitative small-scale explosivity screening: mini-autoclave or ARC with high-speed pressure transducer

https://pubs.acs.org/doi/10.1021/acs.oprd.0c00467

APPLYING O.R.E.O.S. TOOL

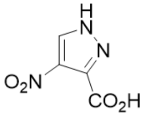
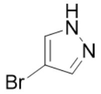
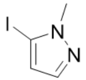
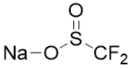
	Points			
	1	**2**	**4**	**8**
Oxygen Balance Hazard		Low	Med	High
Rule of 6 calculation		Pass		Fail
Explosive Functional Group?	No			Yes
Onset temperature	>300	200-300	125-200	<125
Scale	1mg to 5g	5g to 100g	101g to 500g	>500g
O.R.E.O.S. Total:				
		Low Hazard	Medium Hazard	High Hazard
	Points:	7 to 17	18 to 27	28 to 40

High Hazard	• Consider alternative methods.
	• ARC testing is ***required***. -or- • Quantitative small-scale explosivity screening is ***required***
	• Select Test Series 1 is ***required*** based on likely failure mode and available material (Koenen Test, Time/Pressure Test, and/or U.N. Gap)

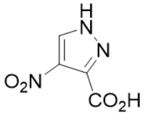
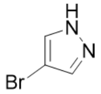
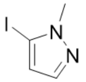
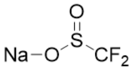
Quantitative small-scale explosivity screening: mini-autoclave or ARC with high-speed pressure transducer

https://pubs.acs.org/doi/10.1021/acs.oprd.0c00467

APPLYING O.R.E.O.S. TOOL

Entry	Material	OB	Rule of 6	ExFG	Onset	1mg to 5g	5g to 100g	101g to 500g	>500g
1	 4-nitro-3-pyrazolecarboxylic acid	High (8)	Fail (8)	Yes (8)	200-300 (2)	Medium Hazard	High Hazard	High Hazard	High Hazard
2	 4-bromopyrazole	High (8)	Fail (8)	Yes (8)	>300 (1)	Medium Hazard	Medium Hazard	High Hazard	High Hazard
3	 5-iodo-1-methylpyrazole	High (8)	Fail (8)	Yes (8)	200-300 (2)	Medium Hazard	High Hazard	High Hazard	High Hazard
4	 sodium difluoromethane-sulfinate	High (8)	Pass (2)	No (1)	125-200 (4)	Low Hazard	Low Hazard	Medium Hazard	Medium Hazard

APPLYING O.R.E.O.S. TOOL

Entry	Material	OB	Rule of 6	ExFG	Onset	1mg to 5g	5g to 100g	101g to 500g	>500g
1	 4-nitro-3-pyrazolecarboxylic acid	High (8)	Fail (8)	Yes (8)	200-300 (2)	Medium Hazard	High Hazard	High Hazard	High Hazard
2	 4-bromopyrazole	High (8)	Fail (8)	Yes (8)	>300 (1)	Medium Hazard	Medium Hazard	High Hazard	High Hazard
3	 5-iodo-1-methylpyrazole	High (8)	Fail (8)	Yes (8)	200-300 (2)	Medium Hazard	High Hazard	High Hazard	High Hazard
4	 sodium difluoromethane-sulfinate	High (8)	Pass (2)	No (1)	125-200 (4)	Low Hazard	Low Hazard	Medium Hazard	Medium Hazard

Allows for prioritization of testing

APPLYING O.R.E.O.S. TOOL

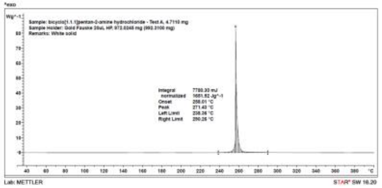
Incorporate into eLN!

T(onset) Threshold (°C)	105.1
Max Energy (J/g)	-1257
Thermal Risk	Very High (>1000 J/g)
Potentially Shock Sensitive	Yes
Potentially Explosive	Yes

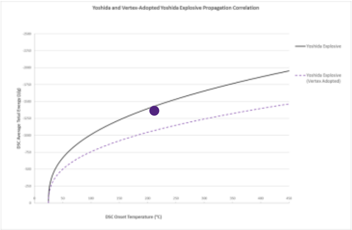
Chemical	OB	Rule of 6	ExFG	Onset (°C)	Scale			
					<5g	5g to 100g	>100g to 500g	>500g
Azobisisobutyronitrile (AIBN)	Med (4)	Pass (2)	Yes (8)	<125 (8)	Medium Hazard	Medium Hazard	Medium Hazard	High Hazard

CONCLUSIONS

- U.N. methods for classification of explosives are complex and material intensive
- Screening methods are convenient, but path forward is unclear when potential risk identified
- Vertex has developed a tool that combines the oxygen balance calculation, "rule of six", the ExFG list, the onset of decomposition by DSC, and the proposed scale into the O.R.E.O.S. assessment
- O.R.E.O.S. tool provides consistency when evaluating compounds that may possess explosive properties and provides recommendations for process safety testing
- O.R.E.O.S. is fully customizable to meet companies' internal guidance for handling energetic compounds



DSC data



Yoshida Correlation

	Points			
	1	2	4	8
Oxygen Balance Hazard		Low	Med	High
Rule of 6 calculation		Pass		Fail
Explosive Functional Group?	No			Yes
Onset temperature	>300	200-300	125-200	<125
Scale	1mg to 5g	5g to 100g	101g to 500g	>500g
O.R.E.O.S. Total:				
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Points:		7 to 17	18 to 27	28 to 40

O.R.E.O.S. Tool

Process Safety testing recommendations

Sperry, J.B.; Azuma, M.; Stone, S. *Org. Process Res. Dev.*, ***2021***, *2, 212-224*

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- Michael Azuma
- Connor Barrett
- Shane Stone

Email: Jeffrey_Sperry@vrtx.com

