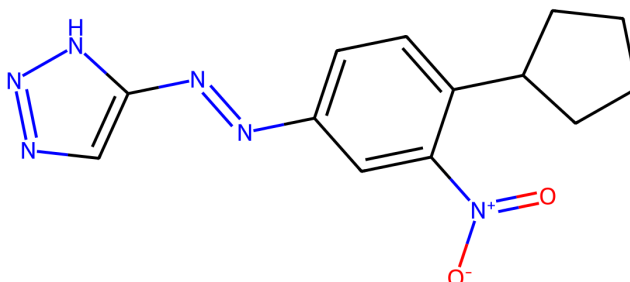


# Thermal Hazard Assessment Memo

## TestMol



## Molecule Properties

SMILES: O=[N+]([O-])c1cc(/N=N/c2cnn[nH]2)ccc1C1CCCC1

Formula: 13C, 14H, 6N, 2O

MW: 286.30 g mol<sup>-1</sup>

mp: 111.0 to 113.0 °C

## Results

High Energy Groups: (3) N1C=CN=N1 |c:1,3|, CN=NC, C[N+](=O)[O-]

Explosive Groups: (3) CN=NC, N1C=CN=N1 |c:1,3|, C[N+](=O)[O-]

Rule of Six = 5                      Oxygen Balance = -173.25

Q<sub>DSC</sub> = 660.0 J g<sup>-1</sup>                      T<sub>onset</sub> = 330.0 °C                      T<sub>init</sub> = 440.0 °C

Impact Sensitivity = -0.12                      Explosive Propagation = -0.18                      T<sub>D24</sub> = 262.0 °C

O.R.E.O.S. assessment of risk by scale:

<5 g	5 to 100 g	100 to 500 g	>500 g
Medium Hazard	Medium Hazard	Medium Hazard	High Hazard

## Interpretation

The 'Rule of Six'<sup>1</sup> is a simple metric that checks if there are at least 6 times as many carbon atoms as there are high energy functional groups in a molecule. The result above shows the result shows the difference between 6 times the number of high energy groups vs the number of carbon atoms. As such a value of  $\leq 0$  implies that a compound should be safe to handle. Here the compound was found to be **(Explosive)** by this metric.

The 'Oxygen Balance'<sup>1</sup> is a method for assessing the explosive properties of molecules. The value is based on the carbon, hydrogen and oxygen content of a molecule and the MW. Using the oxygen balance the explosive risk can be assessed as 'High (OB -120 to 80)', 'Medium (OB 80 to 160, or -240 to -120)', or 'Low' (OB  $<-240$  or  $>160$ ). Here the risk is assessed as **(Medium Risk)**.

The likelihood that a compound would exhibit impact sensitive or explosive propagation can be estimated from their 'Yoshida values'. These Yoshida values have been calculated using the Pfizer method from the  $Q_{DSC}$  and  $T_{onset}$  data.<sup>2</sup> If the Yoshida values are  $<0$  the compound is not expected to exhibit that property. Here the molecule is expected to **not be impact sensitive** and to **not exhibit explosive propagation** based on these values.

$T_{D24}$  is the temperature at which the time to the maximum rate of a runaway reaction is 24 h.<sup>3</sup> A reaction where the time to maximum rate is  $\geq 24$  h is highly unlikely to develop a thermal runaway. As such a reaction temperature of **262.0 °C or below** would be considered appropriate for this compound.

The O.R.E.O.S. assessment method assigns points based on the Oxygen Balance, Rule of 6 value, presence of Explosive functional groups, Onset temperature ( $T_{onset}$ ), and reaction Scale.<sup>1</sup> As such two different point scales are used depending on if an onset temperature is provided or not. Including  $T_{onset}$  data from DSC measurement is preferred. The table above provides the risk categories determined for this compound at 4 different scales. Low Hazard results indicate reactions that can be performed using only the standard precautions. For use of compounds at scales that indicate Medium or High risk, discussion must be first had with the process safety team prior to any further action. The O.R.E.O.S. value score for each scale was found to be:

<5 g	5 to 100 g	100 to 500 g	>500 g
22	23	25	29

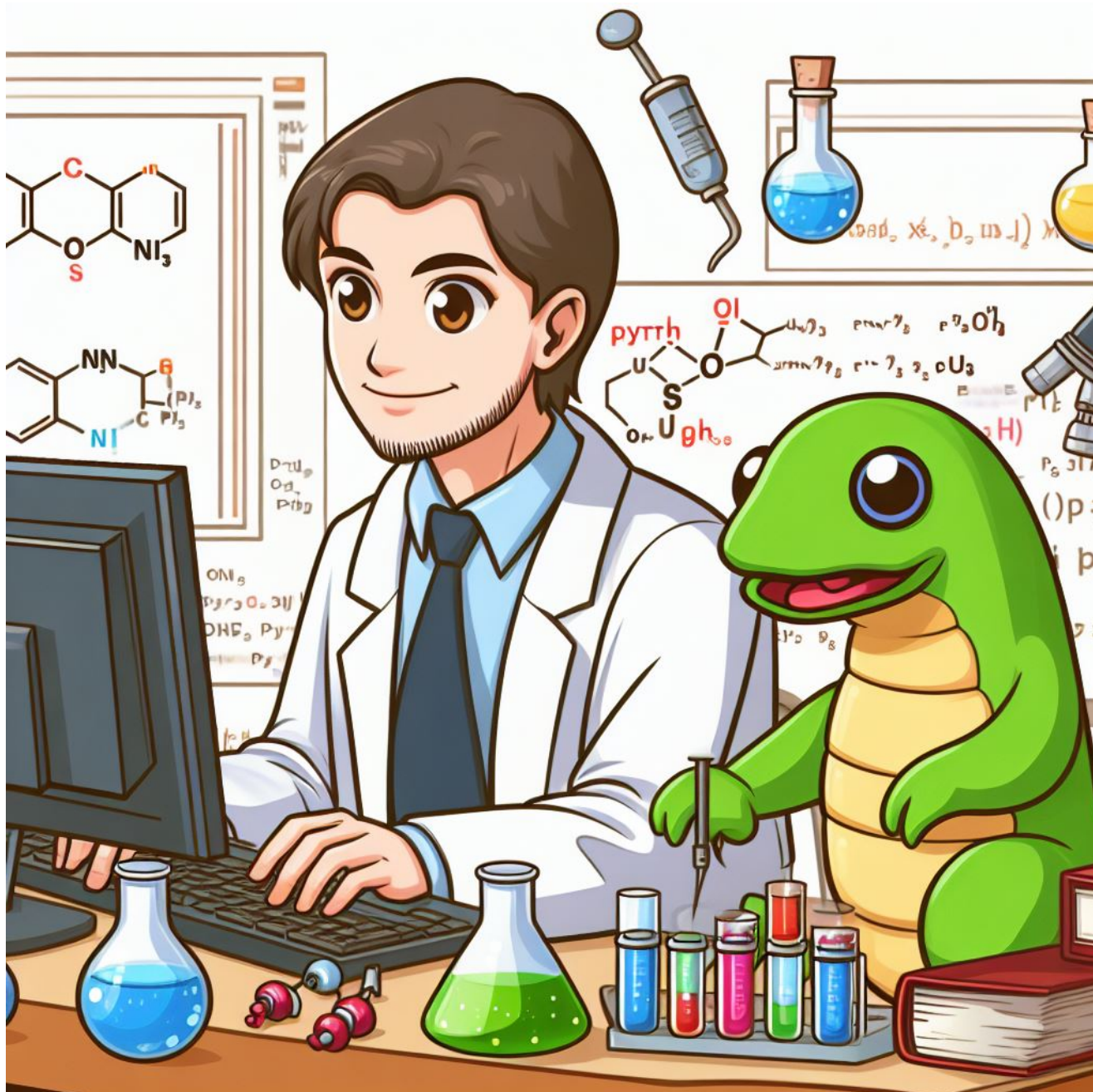
[1]: *Org. Proc. Res. Dev.*, 2021, 25, 2, 212-224

[2]: *Org. Proc. Res. Dev.*, 2020, 24, 1, 67-84

[3]: *Angew. Chem. Int. Ed.*, 2020, 59, 15798-15802

## Additional Data

Git3.jpg



This memo may contain confidential information.

[ThermalDex](#)