Highly efficient and stable peracid for rapid and selective oxidation of aliphatic amine to oxime

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DSC analysis of dodecanebis(peroxoic acid)

1. **Instrument**
   
   DSC Q100 V9.9 Build 303 (Universal V4.5A TA Instrument)

2. **Operation conditions**
   
   **Ramp**: 10.00 °C/min to 300.00 °C
   
   **Gas**: Nitrogen
   
   **Flow rate**: 50.0 ml/min
   
   **Sample weight**: 2.30 mg

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**Fig. 1. DSC analysis of dodecanebis(peroxoic acid)**

**Yoshida’s correlation equations**:

1. **Shock Sensitivity (SS)**

   \[
   \text{SS} = [\log (Q_{dsc}) - 0.72] [\log (T_{dsc} - 25) - 0.98]
   \]
2. Explosion Propagation (EP)  

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

\[ Q_{dsc} = \text{Energy of the exotherm in calories/g} \quad = 1478 \text{ J/g} = 0.0003530 \text{ calories/g} \]

\[ T_{dsc} = \text{The onset temperature of the exotherm in °C} \quad = 100.61 \text{ °C} \]

**Calculations:**

1. **Shock Sensitivity (SS)**

\[ SS = \log(Q_{dsc}) - 0.72 \times \log(T_{dsc} - 25) - 0.98 \]
\[ = \log(0.0003530) - 0.72 \times \log(100.61 - 25) - 0.98 \]
\[ = -4.1722 \times 0.8985 \]
\[ = -3.7490 \]

2. **Explosion Propagation (EP)**

\[ EP = \log(Q_{dsc}) - 0.38 \times \log(T_{dsc} - 25) - 1.67 \]
\[ = \log(0.0003530) - 0.38 \times \log(100.61 - 25) - 1.67 \]
\[ = -3.8322 \times 0.2085 \]
\[ = -0.7993 \]

**Conclusion:**

“According to this equation, if the value for Shock sensitivity (SS) or Explosion Propagation (EP) is \( \geq 0.00 \), then the material is predicated to be shock sensitive or demonstrate explosive propagating properties, respectively.”

As per the above assumption, it is clear that, dodecanbis(peroxoic acid) is non-shock sensitive as well as it does not exhibit explosive propagation properties.

**Reference**

1H-NMR-Spectra of Selected Compounds

1. Benzaldehyde oxime (2a)
2. 2-methoxybenzaldehyde oxime (2b)
3. 3-methoxybenzaldehyde oxime (2c)
4. 4-methoxybenzaldehyde oxime (2d)
5. 3-nitrobenzaldehyde oxime (2f)
6. 4-nitrobenzaldehyde oxime (2g)
7. 4-chlorobenzaldehyde oxime (2h)
8. 4-fluorobenzaldehyde oxime (2i)
9. Acetophenone oxime (2k)
10. 4-hydroxybenzaldehyde oxime (2m)
11. 1-naphthaldehyde oxime (2n)
12. Cyclohexanone oxime (2p)