

1 **Molecular Design of Long Intra-annular Nitrogen Chains : 3H-**
2 **tetrazolo[1,5-d]tetrazole-Based High-Energy-Density Materials**

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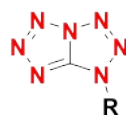
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|---|-------------------|---|---------------------|
| 1 | R=H | 5 | R=NF ₂ |
| 2 | R=NH ₂ | 6 | R=CN |
| 3 | R=NO ₂ | 7 | R=ONO ₂ |
| 4 | R=N ₃ | 8 | R=NHNO ₂ |

Figure 1. 3H-tetrazolo[1,5-d]tetrazole and its derivatives

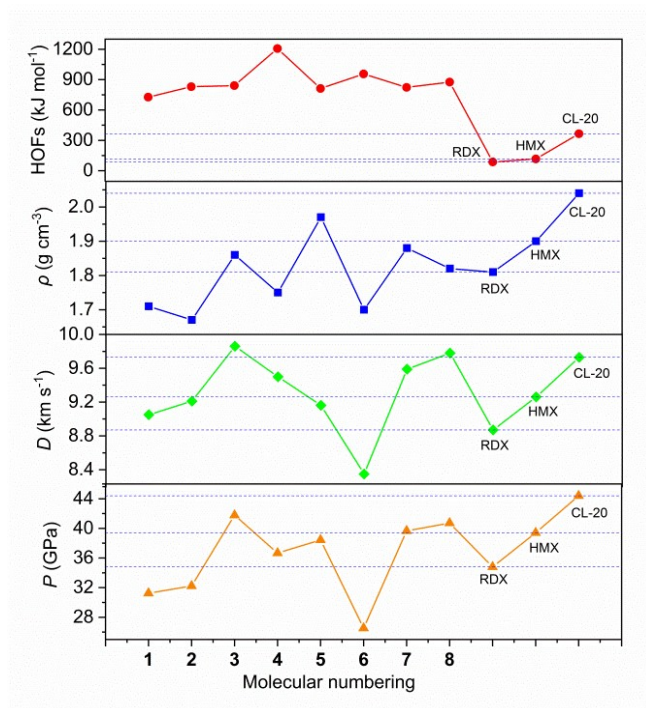


Figure 2. The comparison for density, HOF, P and D of 1-8, RDX, HMX, and CL-20

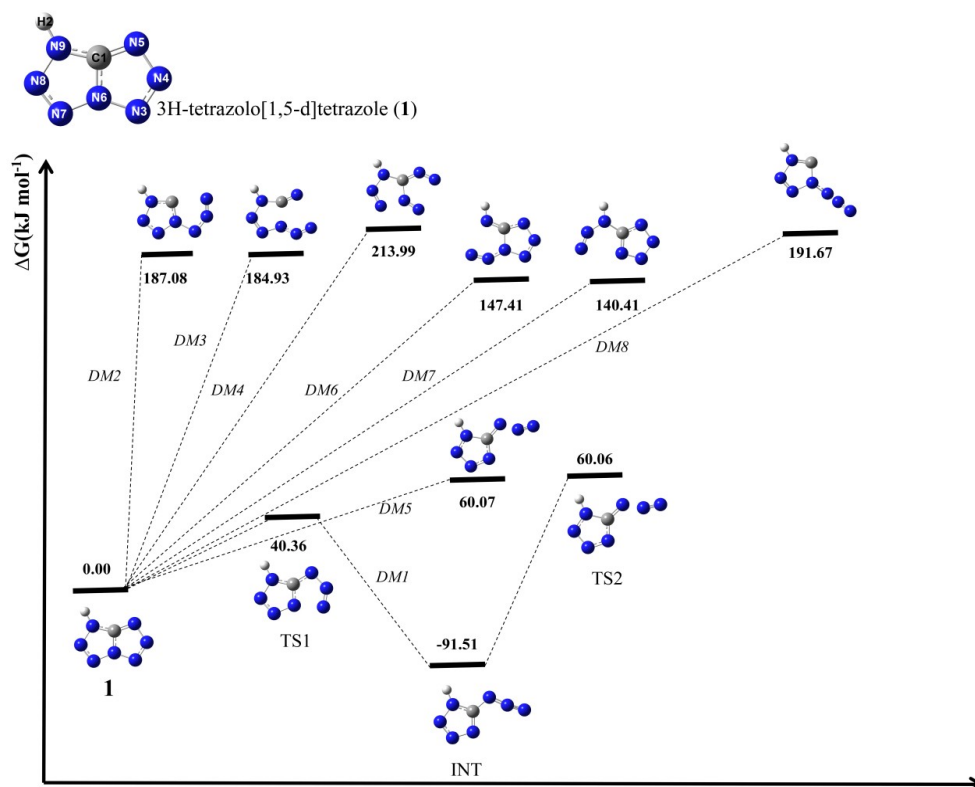


Figure 3. The possible decomposition pathways of compound 1

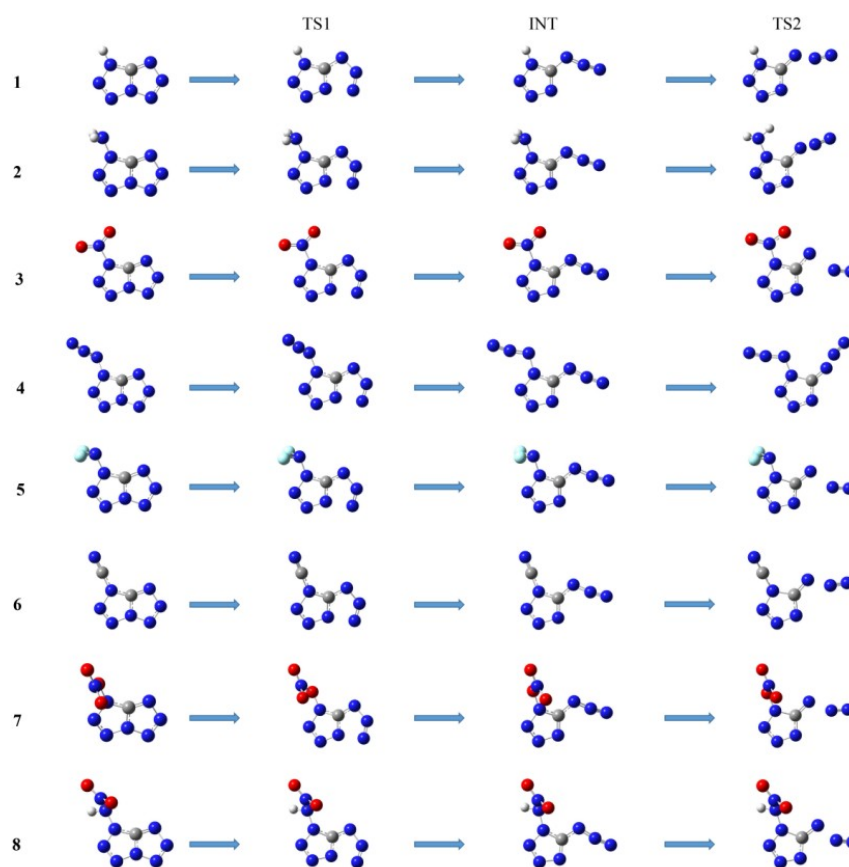


Figure 4. The most likely decomposition pathways of compounds 1-8