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Ab initio molecular dynamics simulations on sensitivity of nitrogen-rich poly-tetrazolo energetic compounds ANGUANG HU, FAN ZHANG, Defence Research and Development Canada-Suffield, PO Box 4000, Stn Main, Medicine Hat, AB, T1A 8K6 Canada — Polyazido nitrogen-rich heterocyclic energetic compounds have gained attention recently due to their high heats of formation and less hazardous effects on the environment. These compounds are generally featured with C-N binary nitrogen-rich heteocycles. It was also found that they may serve as precursors for the preparation of carbon nanotubes and nitrogen-rich carbon nitrides. However, these high energetic compounds can be extremely sensitive to shock, friction, impact, and electrostatic discharge. In the present paper, an azide-tetrazole chain-ring tautomerism was proposed to form new compounds structured with tetrazole rings. The sensitivity and the heats of formation for these poly-tetrazolo compounds have been investigated using *ab initio* quantum chemistry and *ab inito* biasing potential molecular dynamics simulations. The results have shown that these poly-tetrazolo compounds are potentially new, environmentally friendly and high-performance energetic materials that are characterized with low sensitivities and good thermal stabilities.

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