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Molecular Mechanisms in the shock induced decomposition of FOX-7

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TEAM — Experimental and first principle computational studies on FOX 7 have
either involved a very small system consisting of a few atoms or they did not take
into account the decomposition mechanisms under extreme conditions of tempera-
ture and pressure. We have performed a large-scale reactive MD simulation using
ReaxFF-lg force field to study the shock decomposition of FOX 7. The chemical
composition of the principal decomposition products correlates well with experi-
mental observations. Furthermore, we observed that the production of N$_2$ and H$_2$O
was inter molecular in nature and was through different chemical pathways. More-
over, the production of CO and CO$_2$ was delayed due to production of large stable
C,O atoms cluster. These critical insights into the initial processes involved in the
shock induced decomposition of FOX-7 will greatly help in understanding the factors
playing an important role in the insensitiveness of this high energy material.

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