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# Quantum mechanical study of (PAN) $BrCH_2C(O)OONO_2$

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Peroxycarboxylic nitric anhydrides (PANs) are among the most important organic compounds in the atmosphere. PANs are formed in the atmosphere through the same chemistry, involving volatile organic compounds (VOCs) and oxides of nitrogen ($NO_x$), that forms ozone ($O_3$). As such they are excellent indicators of the extend of VOC-$NO_x$ photochemistry, and the relative abundance of the different PAN compounds contains information in the mixture of VOCs that was involved in the $O_3$ formation process. PAN is the most abundant odd nitrogen ($NO_y$) species in this environment. As a $NO_x$ reservoir compound it has the ability to transport $NO_x$ to remote environments, allowing for $NO_x$ photochemistry and/or deposition of nitrogen to these clean locations.
Brominated PAN, $BrCH_2C(O)OONO_2$ (Peroxybromoacetic Nitrate), like other brominated species, is very important in atmospheric chemistry since it may release Br atoms that affect ozone depletion cycles. The compound has never been characterized theoretically before although such a study is very significant in investigating its reactivity in the environment.
In the present work, we have carried out the quantum mechanical study of this compound, using high level theoretical techniques. Electronic molecular structure optimizations and harmonic vibrational frequency calculations performed using the Gaussian 98 series of programs at the restricted MP2 and B3LYP levels of theory. Both optimizations have given comparable results. To refine the energetics of the overall system CBS single point energy calculations have been made at the B3LYP optimized geometries.
Finally the thermochemistry of $BrCH_2C(O)OONO_2$ has been considered