GAS PHASE STRUCTURE OF TRIFLUOROACETYL PEROXYNITRATE.

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The molecular structure and conformational properties of trifluoroacetyl peroxynitrate, FPAN, $CF_3C(O)OONO_2$, were investigated in the gas phase by electron diffraction, microwave spectroscopy and quantum chemical methods. All experimental and theoretical methods show the syn conformer (C=O bond of the acetyl group syn to O-O bond) to be strongly predominant relative to the anti conformer. The O-N bond is extremely long (1.526 (10) Å), which correlates with the low bond energy and the easy formation of $CF_3C(O)OO$ and NO_2 radicals in the atmosphere. The O-O bond (1.408 (8) Å) is shorter than that in hydrogen peroxide (1.464 Å) and the C-O-O-N dihedral angle is close to 85^o.