1,3-Dipolar Cycloaddition of Nitrile Oxides to [C60]fullerene: A Density Functional Theory Study

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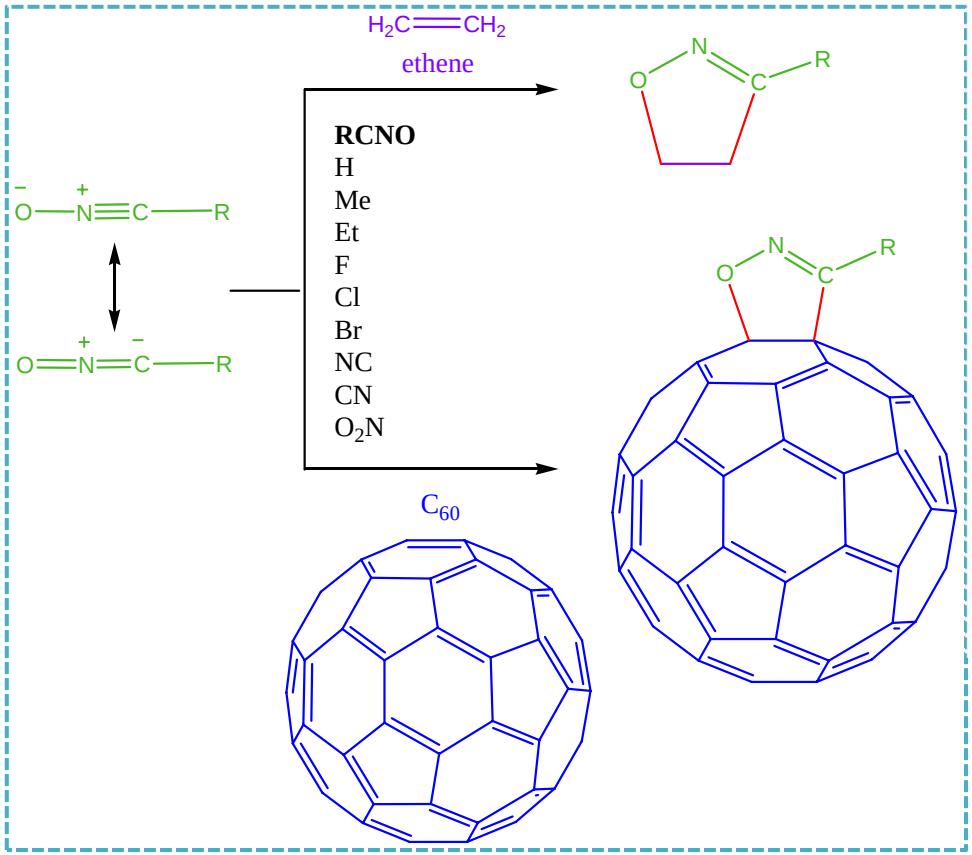
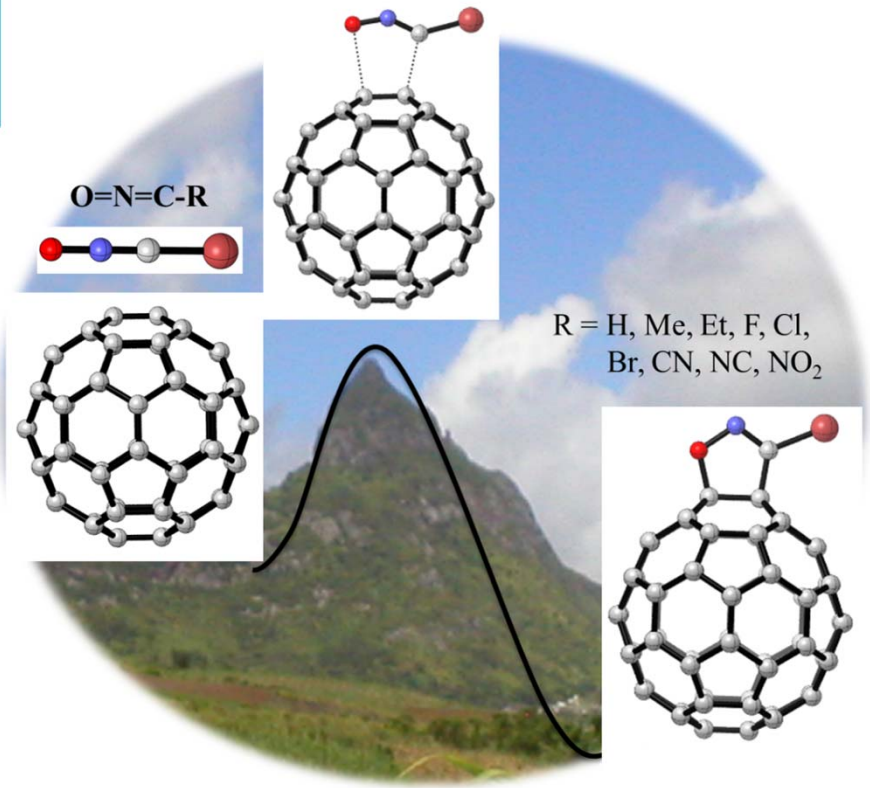
Formation of the monoadducts

The 1,3-DC of unsubstituted and substituted nitrile oxides with electron-releasing and electron-withdrawing substituents with C_{60} is studied by means of B3LYP/6-31G(d) computations. For comparison, the 1,3-DC of these nitrile oxides to ethene have also been studied.





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Formation of the biadducts

The second addition of the **HCNO** to its monoadduct is also considered at the same level of theory.