عنوان مقاله:

The possibility of a two-step oxidation of the surface of C۲۰ fullerene by a single molecule of nitric (V) acid

محل انتشار:

مقالات مروری و پژوهشی شیمی, دوره 2, شماره 1 (سال: 1398)

تعداد صفحات اصل مقاله: 5

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خلاصه مقاله:

p>Oxidation of fullerenes, carbon nanotubes, and graphene, is one of the first proposed and successful approaches > for further functionalization of these nano dimension carbon allotropes. Also, the C۲۰ fullerene, as the smallest known carbon cage, is one of the most important species, in the future of nanotechnology. In this regard, the potential energy surface (PES) study suggests that reaction between nitric (V) acid and C۲۰ fullerene, first leads to the production of a relatively meta-stable kinetically allowed intermediate via a [۲+۳] cycloaddition. After the intermediate is produced, it would subsequently be decomposed to a C۲۰O open-shell fullerene and a HNO۲molecule. Such oxidations were observed via the reaction between strong acids and some of the nano-sized carbon allotropes like carbon nanotube CNTs or spherical fullerenes. The results showed that the produced intermediate directly changes to the final product .of oxidation, in a fast process

کلمات کلیدی:

nitric (V) acid, C۲۰ fullerene, molecular mechanism, PES, reaction channels