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Architecture and Tailoring Of Novel Perfluorinated Molecules and Potential Fire Extinguishants: A Computational Approach

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Opinion

During the past twenty years, it has become widely accepted that the release of constructed halocarbons (halons) into the earth's atmosphere depletes stratospheric ozone. In response to society's concern over the potential effect of ozone depletion, it is being realized world over that in the absence of halons due to Montreal and Kyoto protocol to phase out ozone depletion potential (ODP) and global warming potential (GWP) substances, the search for alternatives begun and which subsequently identified perfluoro compounds as most emerging chemical substitute for halons, therefore perfluorinated analogs and their conjugates are an ideal fire extinguishing agent for industrial applications.[1] Synthetic perfluorinated chemicals in the form of linear/branched/cyclic molecules display interesting fire extinguishing properties.[2] Their efficiency in different systems has emerged with a profile of their potential advantages in industrial and environmental safety applications.

Computational chemistry as a new methodology can explore novel features of perfluorinated compounds with a special focus on molecular modeling for modification in synthetic molecules and their related processes.[3] Different analytical tools for structural analysis of synthesized compounds do not reveal the chemical history and efficacy of the molecule as such therefore a need for a deeper understanding of such molecule is required for developing the best product without wasting extra time and energy. Henceforward, molecular modeling is considered that is a unique technique and applied for evaluating chemical history as well as the efficacy of the proposed molecules to be synthesized in advance. Additionally, the accessible synthetic methods were well-thought-out with some modifications that allow the efficient preparation of offered perfluorinated compounds as per the specific objectives.[4] Perfluorinated compounds are only the alternate solution to replace the ozone depletion potential (ODS) and global warming potential (GWP) agents to protect the environment. Hence, the world scientific community is concentrated mainly on perfluorinated molecules to determine the alternative solution of ODS and GWP culprits.

Therefore, for unique fire extinguishants, different aspects i.e. mathematical and computational models, were conferred, which play a key role in the modeling of these fluorine containing organic frameworks and act as a better option in this research area.[5] Some of the important points to be covered are as (i) design and synthesis of perfluorinated compounds/molecules, (ii) molecular modeling of perfluorinated molecules to be synthesized, (iii) structural characterization of the proposed organic frameworks, (iv) Selective modifications in the skeletons up to the desired lengths, (v) fragments related synthetic protocols, by and establish a structure stability relationship of proposed perfluorinated molecules, (vi) by changing nitrogen as building blocks, (vii) thermal decomposition pathways will also be studied to get information about the structural changes, (viii) to study the GWP effects and impregnating properties.

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Availability of Data and Materials

Wherever necessary, relevant citations are included in the reference section. The author has divided the reference section into two-part, scientific references, and non-scientific references to avoid confusion.

Competing Interests

The author has declared that no competing interest exists.

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