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The extraordinary gravity of three atom 4π -components and 1,3-dienes to $C_{20-n}X_n$ fullerenes; a new gate to the future of Nano technology

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Abstract: A quick glance to the adsorption, sensing, and energy storage abilities of C_{20} fullerene and its derivatives indicate that this small carbon cluster may have extraordinary properties which would make it a key part of the future of Nano actuators and Nano machines. For example, in the case of the gravity of three atom 4π -components (TACs) to these carbon cages, it should be noted that; the rate constants (K)s of the reaction of C_{20} fullerene with 1,3-butadiene (Diels-Alder (DA) process), and with 2-furan nitrile oxide ([3+2] cycloaddition (32CA process)) are $2.51(10^{11}) M^{-1} s^{-1}$, and $1.4(10^7)M^{-1} s^{-1}$, respectively. However, the rate constant of the 32CA reaction between norbornadiene and 3,4-dihydro isoquinoline-N-oxide is about $2.56(10^{-5}) M^{-1} s^{-1}$ (both by DFT and by experimental results). This simple comparison could show the extraordinary gravity of some TACs and dienes to C_{20} fullerenes.

Keywords: [3+2] cycloadditions, Nano technology, C_{20} fullerene, actuators, reaction mechanism, functionalization

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Introduction

It is generally accepted that the catalyst aided [3+2] cycloaddition (32CA) reaction is a powerful tool for synthesizing different types of heterocyclic small molecules, and bioactive or pharmaceutical drugs [1-5]. This reaction was designed as a catalyst-free approach at

firsts [6-8]. However, in most of the cases, the rate as well as the yield of the reaction was low [9-17]. Beside this, there is a concern of emergence of different impurities with high percentage during this reaction in absence of catalysts. Indeed, in a catalyst-free 32CA process, the relative substituents configuration within addends moieties, stereospecificity is lost, when the mechanism turns from a one-step route to a stepwise one. Subsequently, parallel reaction channels leading to the emergence of stereoisomers and some other impurities will be opened [18-20]. Obviously, such problems in the stepwise routes are the result of emergence the diradical or zwitterionic acyclic intermediates.

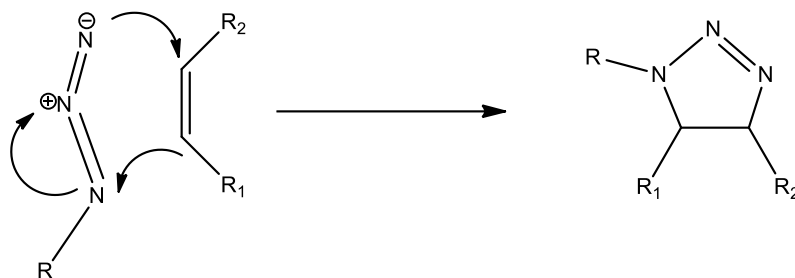
In one hand, the use of catalysts for 32CA process results in some benefits like higher reaction rate, more yield, with higher purity in view of stereoisomers. On the other hand, it might bring some concerns like the need of preparative or flash chromatography, (especially in the case of metal organic complexes), and more cost (due to the need of applying more expensive complexes and solvents) [21-24]. Thus, choosing the reagents and the procedures for scheming a 32CA reaction have always been challenging for researchers [25-27].

In the recent decades, the knowledge of mankind about Nanotechnology has been widely changed. Somehow, with the aid of this interesting field, significant improvements in different areas such as computer systems, communications, and even space machines have occurred [28-30]. Actually, functionalization of nano particles, is one of the most important requirements for development of nanotechnology [31,32]. Thus, many precious attempts have been done by scientists to reach to this goal [33-35]. Researches were ongoing until in some of the recent reports, an extraordinary tendency of some fullerene especially the smallest one (C_{20} fullerene and its derivatives, to three atom $4n$ -components (TACs) or dienes were observed [36-40]. In this paper, these reports about such attraction have been reviewed, in a quick glance.

A brief history of [3+2] cycloadditions

To the best of our knowledge, the first reports about the TACs comes back to 1883, discovering the diazoacetic ester by Theodor Curtius [41]. Also, the first 32CA reaction was reported by Buchner (a member of Curtius' group) in 1888 [42]. He reacted methyl acrylate with methyl diazoacetate. Then, he successfully isolated 2-pyrazoline which was formed by the rearrangement of initially formed 1-pyrazoline. Five years later, Ueber [43], and Pechmann [44], reported two new 32CA reactions by alkyl azides, and diazoalkanes, respectively. In 1890s, Beckmann [45], and Werner - Buss (1894) [46] discovered azomethine oxides (nitrones), and nitrile oxides, respectively. About, forty years later (1938), Smith published the first review article about 32CA, introducing this reaction as a new

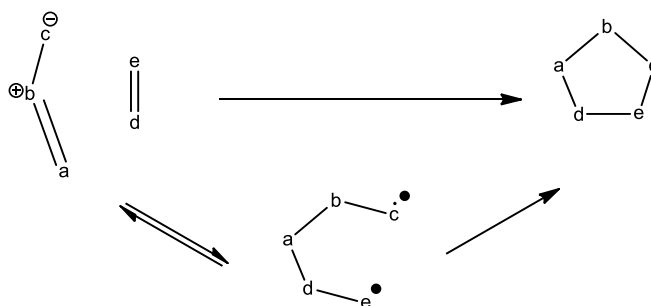
approach for synthesizing five-membered ring heterocyclic compounds [47]. However, the use of this reaction as an approach of synthesis was thought to be limited [48]. Subsequently, several researchers focused on synthesizing heterocyclic compounds via 32CA reactions [49,50]. For example, Rolf Huisgen published a number of reports about the 32CA reaction as a powerful tool for synthesizing heterocycles [51,52]. Moreover, he classified TACs and the 32CA processes [53].



Scheme 1. Huisgen's "concerted" mechanism for 32CA reaction

The first proposals about the mechanistic aspect of the 32CAs were made by Huisgen in 1960's decade, along with the synthetic investigations on it. In his paper, he suggested a single-step one-step mechanism (Scheme 1) for the reaction which made that stereospecific [54]. Huisgen's theory about the 32CA reaction mechanism was supported by Woodward–Hofmann's theory about pericyclic reactions [55], and it was further aided by Fukui's theory defining the Frontier Molecular Orbitals (FMOs) [56] and recently by the molecular electron density theory (MEDT) [57].

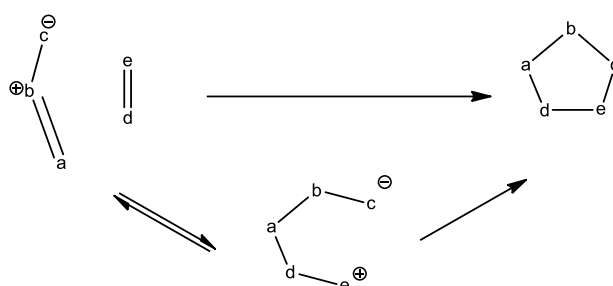
In 1968, Raymond Firestone suggested another mechanism for the process that was in contrast with Huisgen's theory [58]. Firestone hypothesized that this reaction proceeds via a diradical intermediate (Scheme 2) leading the reaction to be stepwise [58–60]. Subsequently, in 1976, Huisgen published a review article entitled "*Concerted nature of 1,3-dipolar cycloadditions and the question of diradical intermediates*" that insisted on the one-step nature of the reaction mechanism [61].



Scheme 2. Firestone's diradical mechanism for 32CA reaction

Then, Kendall Houk in cooperation with Firestone at 1985, emphasized that an experimental example of 32CA reaction was stereospecific indicating that the reaction mechanism was one-step [62].

During decades, scientists continuously reported the examples of this reaction with stereospecific outcomes supporting the one-step mechanisms [63–65]. After those reports, the mechanism of 32CA was mainly accepted to be asynchronous one-step [66]. Finally, in 1986, Huisgen and Mlostoń discovered that in the case of the 32CA reaction between an electron-rich thiocarbonyl ylide and a highly electron-poor tetracyanoethene, the reaction could proceed via a zwitterionic intermediate route (Scheme 3) dividing the reaction into a two-step one [67,68].



Scheme 3. The Stepwise mechanism through the zwitterionic intermediate

After those reports about that interesting issue, attempts to find more examples of two-step 32CAs were made; however, most of the reported examples referred to thiocarbonyl ylides [69–71]. Also, it should be noted that in some especial cases, stepwise 32CA processes using the other TACs were observed. Sauer (in 1999), for instance, reported a non-stereospecific 32CA reaction of a group of azomethine ylide derivatives and enamines [72]. As another example, Luis Domingo (in 2004) presented an example of a 32CA reaction in which both stepwise and one-step pathways were in a close competition [73]. Moreover, Kuznetsov (2006), published a comprehensive review paper in which several reports about the 32CAs were discussed [74].

In the recent years, hot debates on the mechanism of 32CA raised, due to the importance of the stereospecificity of this process. For instance, in 2013, Firestone used some examples with strong reasoning and reiterated that the 32CA process might be a two-step diradical one [75]. Jasiński found that the 32CA reaction between a highly electro-negative dinitro alkene (gem-dinitroethene) and a nitron with a high potentially resonance-stabilizing structure [(Z)-C,N-diphenylnitron] was stepwise in toluene as solvent [76]. Mlostoń (2015) introduced two new experimental examples of diradical 32CAs [77,78], and in some other reports, we have published examples of three-steps zwitterionic 32CA reactions [79,80]. Today, numerous examples by different scientists all around the world, show that the

concern of emergence of stereo impurities via the stepwise pathways for the 32CA processes is real [81-100]. Moreover, the accuracy of theoretical studies on the mechanism and kinetics of 32CA process have been confirmed by comparative quantum chemical investigations [101-115].

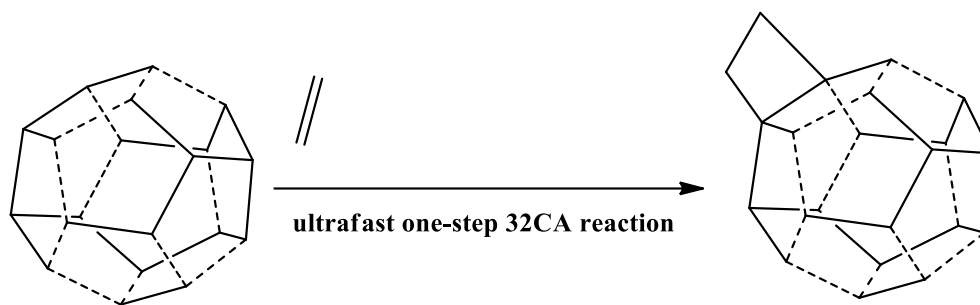
Current application of C₂₀ fullerenes

C₂₀ fullerene is the smallest known carbon cage which has been firstly hypothesized by scientists like Wahl et al. [116], Ke et al. [117], and Taylor et al [118]. Then, reports about its gas phase synthesis were revealed by researchers like Prinzbach in Nature magazine at 2000 [119], or Podlivaev [120]. After that, studies on the stability [121-124] of this cluster were performed. Also, in parallel with those studies, investigations on the other properties of this small carbon cage, such as its electronic [125], magnetic moment formation [126], its memory effects on the other surfaces [127], energy storage [128], electron transport [129], and optoelectronic behavior [130] were performed. Moreover, Baei's works [131,132] and Siadati et al systematic studies on especial adsorption [37-40], sensing [133-136], and nano-sized actuating applications [137] might be of important reports in this especial field. However, there are several precious investigations on the adsorption [138-141], and sensor application [142-147] of this smallest carbon cage, by other researchers.

A quick glance to the adsorption, sensing, and energy storage application of C₂₀ fullerene and its derivatives indicate that this small carbon cluster may have extraordinary properties which would make it a key part of the future nano actuators and machines. Also, the powerful gravity of this into the dipoles as well as dienes leads to a fast and facile catalyst-free cycloaddition between these species. It seems that such facile functionalization in one hand and the especial electronic properties on the other hand; make it the candidate for advancing the field of nano technology.

Examples of fast functionalization of C₂₀ fullerenes by [3+2] cycloadditions

As mentioned before, the yields and the reaction rate parameters (like the rate constant) of usual 32CAs are low (especially in absence of catalysts). But the products of this reaction are precious due to formation of new five-membered rings. Many attempts have been made to improve the reaction rate and yield; while, in most cases, researchers have been forced to use different types of catalyst. Thus, in the case of functionalization of C₂₀ fullerene family by the 32CA (Scheme 4), the interesting point is; that the reaction rate (and other thermodynamic and kinetic parameters) are extremely high.

Scheme 4. The ultrafast 23-DC reaction between the C₂₀ fullerene and alkenes

That is, we suggest that the 32CA (as well as DA reaction) become a candidate for usual and experimental functionalization of fullerenes (especially C₂₀ fullerene family). Table 1, presented some of the experimental as well as theoretical data of the usual 32CA reactions in comparison of theoretical results for 32CA process on C₂₀ fullerene family.

Table 1. The key thermodynamic and kinetic parameters for reactions with the participation of C₂₀ fullerene.

Entry	Unsaturated	TAC or diene	ΔG^\ddagger (kcal mol ⁻¹)	K (M ⁻¹ s ⁻¹)	ΔH^\ddagger (kcal mol ⁻¹)	ΔS^\ddagger (kcal mol ⁻¹ K ⁻¹)	Ref
1	C ₂₀	1,3-butadiene	1.89	2.51(10 ¹¹)	11.60	-3.26(10 ⁻²)	[36]
2	C ₂₀	4-pyridine nitrile oxide	9.09	1.03(10 ⁶)	2.63	-21.6(10 ⁻³)	[37]
3	C ₂₀	2-furan nitrile oxide	13.3	1.1(10 ³)	5.41	-2.47(10 ⁻²)	[38]
4	C ₂₀	2-furan nitrile oxide (7.96	1.4(10 ⁷)	2.41	-1.86(10 ⁻²)	[38]
5	C ₁₈ NB	4-pyridine nitrile oxide)	14.60	1.19(10 ²)	11.20	-11.6(10 ⁻³)	[39]
6	C ₂₀	HNO ₃	17.40	-	14.70	-	[40]
7	C ₂₀	Benzene	21.72	7.42(10 ⁻⁴)	14.29	-	[148]
8	B ₁₂ N ₁₂	Methyl azide	16.75	5.25(10 ¹)	10.21	-21.94(10 ⁻³)	[151]
9	C ₂₀	HCNO	12.48	3.76(10 ²)	2.64	-4.10(10 ⁻²)	[152]
10	C ₂₀	HN ₃	15.77	2.14	4.79	-4.70(10 ⁻²)	[152]
11	N-ethylmaleimide	Benzonitrile oxide	17.60 (DFT) 17.82(exp)	-	17.90	-1.0(10 ⁻³)	[106]
12	ethyne	azide	25.5 (DFT) 25.2(exp)	-	22.40	-10.7(10 ⁻³)	[109]
13	Norbornadiene	3,4-dihydro iso-quinoline-N-oxide	23.7 (DFT) 23.7(exp)	2.56(10 ⁻⁵)	22.90	-2.1(10 ⁻³)	[110]

At the first glance to Table 1, two issues could be clearly concluded. The first one is the accuracy of the theoretical calculation (the very good agreement between experimental and

theoretical results). For example data in entries 11 to 13 show that the results of DFT method for the Gibbs free energy are much closed to the experimental outcomes. It could confirm the trustability of such theoretical methods in prediction of kinetics and thermodynamics of 32CA reactions. Also, the second issue is the very slow reaction rates of usual 32CA processes (like $2.56(10^{-5}) \text{ M}^{-1} \text{ s}^{-1}$ in the case of entry 13). But, as given in entries 1 to 10, the rate constant of the reaction between C_{20} fullerene and its derivatives with TACs (especially nitrile oxides compared to azides) are extremely higher compared to the usual unsaturated ones. For example, the rate constant of the reaction of C_{20} fullerene with 1,3-butadiene (entry 1, DA process), and with 2-furan nitrile oxide (entry 4, DC process) are $2.51(10^{11}) \text{ M}^{-1} \text{ s}^{-1}$, and $1.4(10^7)\text{M}^{-1} \text{ s}^{-1}$, respectively; while, the rate constant of the 32CAprocess between norbornadiene and 3,4-dihydro isoquinoline-N-oxide is about $2.56(10^{-5}) \text{ M}^{-1} \text{ s}^{-1}$ (both for DFT and for experimental results). This simple comparison could show the extraordinary gravity of some TACs and dienes to C_{20} fullerenes.

Conclusion

In one hand, several reports during decades confirm that the reaction rates of almost all catalyst-free [3+2] cycloaddition processes are very slow with low yields. On the other hand, the concern of stepwise mechanistic channels leading to emergence of unwanted products makes unfavorable the catalyst-free type of this reaction. That is, most of the practical 32CAs are reported with the aid of catalysts for gaining higher yield and lower impurity profile. But, nowadays, the recent studies show that the especial gravity of C_{20} fullerene (compared to the usual unsaturated bonds) toward TACs or diene species results in very fast 32CA, or DA reactions. For example, the rate constant of the reaction of C_{20} fullerene with 1,3-butadiene (DA process), and with 2-furan nitrile oxide (DC process) are $2.51(10^{11}) \text{ M}^{-1} \text{ s}^{-1}$, and $1.4(10^7)\text{M}^{-1} \text{ s}^{-1}$, respectively. While, the rate constant of the 32CAprocess between norbornadiene and 3,4-dihydro isoquinoline-N-oxide is about $2.56(10^{-5}) \text{ M}^{-1} \text{ s}^{-1}$ (both for DFT and for experimental results). This simple comparison could show the extraordinary gravity of some TACs and dienes to C_{20} fullerenes. Such processes do not require catalysts, heat, or beams of light. Thus, it would be logical that the 32CA, or DA reactions could be a fast, and facile method for functionalization of such carbon based nano sized compounds.

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