Covid-19 Docking Study and Revealing the Various Chemical Reactivity of 1-Bromo(Chloro)-4-vinyl-benzene in [3+2] Cycloaddition Reactions

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Table S1. B3LYP/6-311 G ++ (d,p) total (E, in a.u.) and relative[a] (ΔE, in kcal·mol^{-1}) energies, in gas phase and in THF, for the species involved in the 32CA reaction of 1-bromo-4-vinylbenzene **1** and 1-chloro-4-vinylbenzene **2** with benzonitrile oxide **3**.

	Gas		THF	
System	E	ΔE	E	ΔE
1	-2883.27346555	-------	-2883.27712088	-------
2	-769.353793420	-------	-769.357387799	-------
3	-399.74988687	-------	-399.75663597	-------
1+3	-3283.02335242	-------	-3283.03375685	-------
TS-B-m	-3282.99808619	15.85	-3283.00675874	16.94
B-m	-3283.07352117	-31.48	-3283.08345063	-31.18
TS-B-o	-3282.99271118	19.22	-3283.00085667	20.64
B-o	-3283.06935984	-28.86	-3283.07881597	-28.27
2+3	-1169.10368029	-------	-1169.114023769	-------
TS-C-m	-1169.07833314	15.90	-1169.08694275	16.99
C-m	-1169.15382082	-31.46	-1169.16370578	-31.17
TS-C-o	-1169.07299908	19.25	-1169.08105996	20.68
C-o	-1169.14963979	-28.83	-1169.15899786	-28.22

Table S2. B3LYP/6-311G++(d,p) enthalpies (H, in a.u.), entropies (S, in cal·mol^{-1}·K^{-1}) and Gibbs free energies (G, in a.u.), and relative[a] enthalpies (ΔH, in kcal·mol^{-1}), entropies (ΔS, in cal·mol^{-1}·K^{-1}) and Gibbs free energies (ΔG, in kcal·mol^{-1}), computed at 25 ºC and 1 atm in THF, for the stationary points involved in the 32CA reaction of 1-bromo-4-vinylbenzene **1** and 1-chloro-4-vinylbenzene **2** with benzonitrile oxide **3**.

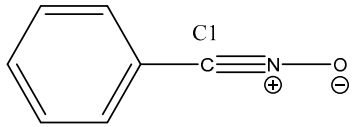
System	H	ΔH	G	ΔG	S	ΔS
1	-2883.145363		-2883.189172		92.204	
2	-769.225257		-769.267631		89.183	
3	-399.645736		-399.686226		85.217	
1+3	-3282.791099	-------	-3282.875398	-------	177.421	-----
TS-B-m	-3282.763611	17.24	-3282.828275	29.56	136.097	41.324
B-m	-3282.836208	-28.30	-3282.898031	-14.20	130.118	47.303
TS-B-o	-3282.757776	20.91	-3282.821086	34.08	133.247	44.174
B-o	-3282.831225	-25.17	-3282.892120	-10.49	128.164	49.257
2+3	-1168.870993	-------	-1168.953857	-------	174.400	-------
TS-C-m	-1168.843466	17.27	-1168.906664	29.61	133.011	41.389
C-m	-1168.916164	-28.34	-1168.977321	-14.72	128.716	45.684
TS-C-o	-1168.837635	20.93	-1168.900129	33.71	131,529	42.871
C-o	-1168.911155	-25.20	-1168.971295	-10.94	126.574	47.826

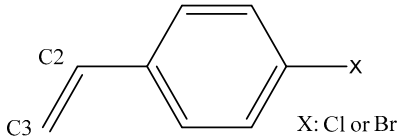
Table S3. ELF topological analysis of the C–C and C–O bond formation along the 32CA reaction between 1-bromo-4-vinylbenzene 2 and benzonitrile oxide 3. Distances are given in angstroms, Å, relative energies in kcal·mol^{-1}, (Relative to reagents).

	B-1	**B-2 TS-B-m**	**B-3**	**B-4**	**B-5**	**B-6**	**B-7**	**B-8**	**B-9**	**B-10**	**B-11**	**B-12**	**B-13**	**B-14**
ΔE	8.37	15.85	15.19	14.65	14.44	14.35	13.73	12.70	7.98	-0.69	-0.99	-9.15	-11.95	-20.50
d (O,C2)	3.254	2.459	2.444	2.407	2.344	2.377	2.359	2.343	2.270	2.140	2.031	1.909	1.846	1.655
d (C1,C3)	3.160	2.177	2.140	2.101	2.031	2.019	1.999	1.959	1.842	1.690	1.621	1.582	1.570	1.543
V(C1,N)	1.75	1.67	1.92	1.93	1.93	1.87	1.87	1.85	1.80	3.32	3.26	3.22	3.21	3.17
V'(C1,N)	1.35	1.46	1.44	1.45	1.46	1.40	1.40	1.38	1.69	-	-	-	-	-
V(N,O)	1.48	1.46	1.45	1.45	1.44	1.41	1.42	1.40	1.37	1.32	1.27	1.22	1.20	1.11
V(C1)	1.50	0.46	0.44	0.42	0.38	0.39	0.37	0.37	-	-	-	-	-	-
V'(C1)	-	0.52	0.58	0.59	0.62	0.72	-	-	-	-	-	-	-	-
V''(C1)	-	0.30	-	-	-	-	-	-	-	-	-	-	-	-
V(N)	1.86	2.10	2.16	2.15	2.18	2.31	2.31	2.36	2.47	2.61	2.67	2.72	2.75	2.82
V(O)	2.60	2.84	2.84	2.83	2.84	2.84	2.84	2.84	2.77	2.84	2.84	2.72	2.67	2.57
V'(O)	3.04	2.79	2.79	2.77	2.76	2.78	2.78	2.77	2.84	2.77	2.78	2.64	2.60	2.50
V''(O)	-	-	-	-	-	-	-	-	-	-	-	0.30	0.39	-
V(C2,C3)	1.66	3.10	3.09	2.86	2.80	2.66	2.64	2.57	2.42	2.31	2.16	2.10	2.08	2.01
V'(C2,C3)	1.58	-	-	-	-	-	-	-	-	-	-	-	-	-
V(C2)	-	-	-	-	-	-	-	-	-	-	-	-	-	-
V(C3)	-	-	-	0.22	0.28	0.38	0.39	-	-	-	-	-	-	-
V(O,C2)	-	-	-	-	-	-	-	-	-	0.12	0.15	0.22	0.25	0.98
V(C1,C3)	-	-	-	-	-	-	0.73	1.24	1.45	1.70	1.81	1.88	1.90	1.95

Table S4. ELF topological analysis of the C–C and C–O bond formation along the 32CA reaction between 1-chloro-4-vinylbenzene 2 and benzonitrile oxide 3. Distances are given in angstroms, Å, relative energies in kcal·mol^{-1}, (Relative to reagents).

	C-1	**C-2**	**C-3 TS-Cm**	**C-4**	**C-5**	**C-5**	**C-7**	**C-8**	**C-9**	**C-10**	**C-11**	**C-12**	**C-13**	**C-14**
ΔE	4.52	12.21	15.85	14.82	10.77	6.46	3.62	0.62	-2.26	-5.03	-16.29	-16.69	-17.00	-28.40
d(C2,O)	2.932	2.632	2.462	2.396	2.356	2.260	2.220	2.177	2.128	2.074	1.821	1.812	1.805	1.492
d(C2,C3)	2.935	2.461	2.177	2.056	1.997	1.816	1.761	1.710	1.666	1.654	1.564	1.564	1.564	1.521
V(C1,N)	3.86	2.23	1.98	1.90	1.84	1.77	1.70	3.37	3.33	3.30	3.21	3.21	3.21	3.13
V'(C1,N)	2.19	1.83	1.46	1.41	1.57	1.69	1.72	-	-	-	-	-	-	-
V(N)	-	1.33	2.08	2.25	2.34	2.49	2.52	2.57	2.60	2.63	2.76	2.76	2.76	2.89
V(N,O)	1.64	1.56	1.47	1.43	1.41	1.37	1.35	1.34	1.31	1.29	1.19	1.18	1.18	1.04
V(C1)	-	0.83	0.50	0.66	-	-	-	-	-	-	-	-	-	-
V(C1)	-	-	0.48	0.41	-	-	-	-	-		-	-	-	-
V(C2)	-	-	-	-	-	-	-	0.18	-	-	-	0.15	0.11	-
V(C3)	-	-	-	0.32	-	-	-	-	-	-	-	-	-	-
V(O)	2.83	2.81	2.83	2.84	2.84	2.84	2.83	2.83	2.84	2.84	2.65	2.67	2.66	2.51
V'(O)	2.82	2.82	2.79	2.77	2.77	2.77	2.77	2.78	2.77	2.79	2.59	2.61	2.60	2.43
V''(O)	-	-	-	-	-	0.32	0.41	0.43		-		-	-	-
V(C2,C3)	1.68	1.69	3.10	2.74	2.63	2.40	2.35	2.32	2.30	2.19	2.07	2.07	2.07	1.96
V'(C2,C3)	1.64	1.56	-	-	-	-	-	-	-	-	-	-	-	-
V(C2,O)	-	-	-	-	-	-	-	-	0.11-	0.15	0.26	0.49	0.54	1.23
V(C1,C3)	-	-	-	-	0.73	1.47	1.57	1.65	1.72	1.78	1.91	1.91	1.91	1.98





1. BET study of the cycloaddition reaction (32CA) of 1-bromo-4-vinylbenzene 1 and 1-chloro-4-vinylbenzene 2 with benzonitrile oxide 3

To better understand bond changes in organic reactions, the theory of bond evolution (BET) is a widely used method [1, 2]. It makes possible to determine the variations in binding along the reaction path and, therefore, to accommodate the nature of the electronic change associated with a given molecular mechanism. Therefore, in order to comprehend the formation of C-O and C-C bonds during the cycloaddtions reactions of 1-bromo-4-vinylbenzene **1** and 1-chloro-4-vinylbenzene **2** with benzonitrile oxide **3**, a BET study along the reaction path meta of these reactions were realized. A representation of the binding changes that take place along the reaction resulting from the ELF topological analysis is shown in Figures S1 and S2.

1.1. ELF topological analysis of the C–C and C–O bond formation along the 32CA reaction between 1-bromo-4-vinylbenzene 1 and benzonitrile oxide 3

So as to explain the C–C and C–O bond formation along the 32CA reaction between 1-bromo-4-vinylbenzene **1** and benzonitrile oxide **3**, a topological investigation of the ELF through the IRC associated with the most favorable *meta* reaction path was executed. The populations of the most relevant ELF valence basins, involved in the formation C–C and C–O single bonds of some selected structures of the IRC are arranged in table S1.

The correlation model obtained from the topological analysis of the ELF of B-1, d(C1-C3)=3.254 Å and d(C-O)=3.160 Å, Can be linked to the electronic structure of the separate reagents.

In the CNO segment of benzonitrile oxide **3**, we observe the presence of two monosynaptic basins, V(O) and V'(O), integrating a total of 5.64e, a disynaptic basin V (N, O), integrating 1.48e, a pair of disynaptic basins, V (C1,N) and V '(C1,N) integrating a total of 3.10e and two monosynaptic basins, V(N) and V(C1), integrating respectively a total of 1.86 and 1.50e. Then again, the C2-C3 double bond of the ethylene segment is characterized by the existence of two disynaptic basins, V(C2,C3) and V'(C2,C3), assimilating a total population of 3.24e. No big changes at **B-2** (TS-B-m), d(C1-C3) = 2.174 Å and d(O-C1) = 2.459 Å except increasing the value of monosynaptic basin V (N) by 0.24e, while the value of monosynaptic basin V(C1) was decreased by 0.24 and the monosynaptic V(C1) basin has been divided into three monosynaptic V(C1), V'(C1) and V''(C1), integrating a total of 1.28e. At **B-3**, d(C1-C3) = 2.140 Å and d(O-C1) = 2.444 Å the only change is that the three monosynaptics V(C1), V'(C1) and V"(C1) have become two monosynaptics V(C1) and V'(C1) integrating a total of 1.02e and the disynaptic basin V(C2,C3) take 3.09e as value.

In **B-4**, d(C1-C3) = 2.101 Å and d(O-C2) = 2.407 Å, the value of the disynaptic basin V(C2, C3) is decreased by 0.23 and the most relevant ELF topological change observed is appearance of a monosynaptic at the carbon C3, V(C3)=0.22e. At **B-5**, d(C1-C3) = 2.031 Å and d(O-C1) = 2.344 Å, the most important change is decrease in the value of the disynaptic basin V(C2, C3) and the increase in the value of the monosynaptic basin V(C3) approximately by 0.6e.

At **B-6**, d(C1-C3) = 2.019 Å and d(O-C2) = 2.377 Å, which is the structure just before the formation of the first C1-C3 single bond, only two monosynaptic basins, V(C1) and V'(C1), integrating 0.39 and 0.72, respectively, are observed and the presence of a new V(C3) monosynaptic basin, integrating 0.38e.

At **B-7**, d(C1-C3) = 1.999 Å and d(O-C2) = 2.359 Å, the two V(C1) and V(C3) monosynaptic basin have merged into a new disynaptic basin V(C1,C3) integrating an initial population of 1.24e. This pertinent topological change can be associated with the formation of the first C1-C3 single bond at a C-C distance of 1.999 Å.

B-10, d(C1-C3) =1.690 Å and d(O-C2)=2.140 Å, which is the structure just before the formation of the second C-O single bond, is characterized by the presence of a V(O,C1) disynaptic basin, integrating 0.12e, At **B-12**, d(C1-C3) = 1.5582 Å and d(O-C2) = 1.909 Å, and At **B-13**,d(C1-C3) = 1.570 Å and d(O-C3) = 1.846 Å, an appearance of a monosynaptic on oxygen is due to the reorganization of free electrons carried by oxygen integrating 0.38e.

As a last point, d(C2–C3) = 1.543 Å and d(O–C1) = 1.655 Å, which corresponds to B-1**4**, the two V(C1,C3) and V(O,C2) disynaptic basins reach populations of 1.95e and 0.98e, respectively. The V(N,O) disynaptic basin ends up with a low population of 1.12e, while the two V(O) and V′(O) monosynaptic basins integrate a total of 5.07e, suggesting a polarised N–O bond. Similarly, the population of the V(C1,N) disynaptic basin is 3.17e, while that of the V(N) monosynaptic basin is 2.82e and the V(C1,C2) disynaptic basin ends up with 2.01e.

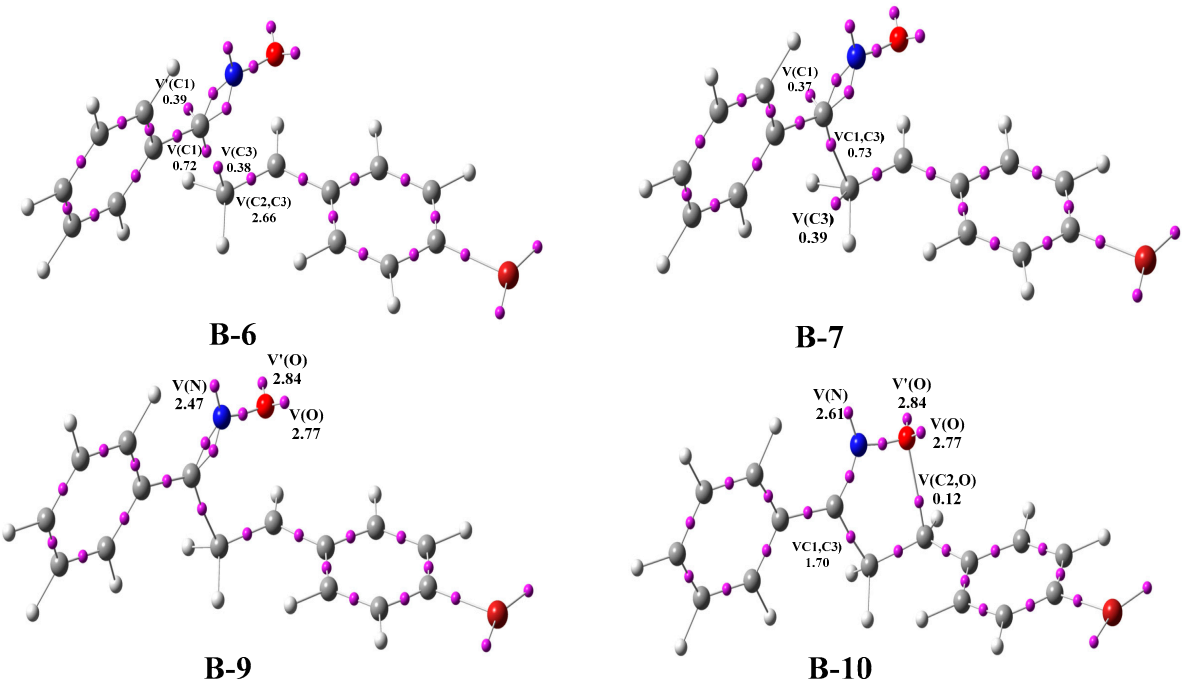


Figure S1. ELF attractor positions for the structures involved in the formation of the C–C and C–O single bonds along the most favorable TS-B-m reaction path associated with the 32CAreaction of 1-bromo-4-vinylbenzene **1** and benzonitrile oxide **3**

1.2. ELF topological analysis of the C–C and C–O bond formation along the 32CA reaction between 1-chloro-4-vinylbenzene 2 with benzonitrile oxide 3

To shed light on the formation of C-C and C-O bonds along the 32CA reaction between 1-chloro-4-vinylbenzene **2** and benzonitrile oxide **3**, a topological scrutinize of the ELF along the IRC associated with the most favorable meta-reaction pathway was performed. The populations of the most relevant ELF valence basins, as well as the C-C and C-O distances of the chosen IRC structures are shown in Table S4.

At **C-1**, d (C2-O) = 2,932 Å and d (C3-C1) = 2,935 Å, the two interacting fragments are very distant from each other, and therefore, the ELF topology of **C-1** is very identical to that noted in the separate reagents. The most important basins are those corresponding to the interacting systems reactive sites, that is to say the bonds C1-N, N-O and C2-C3, the C1-N bond is characterized by the presence of two disynaptic basins V(C1,N) and V'(C1,N), with a population of 3.86 and 2.19e, respectively, indicating the presence of a C3-N triple bond, the N-O bond is characterized by the presence of a disynaptic V(N,O) basin with a population of 1.65e, moreover, the sum of the population of the monosynaptic basins V(O) and V'(O), integrating a total of 5.65e, which shows that the oxygen atom O is negatively charged.

The most important modifications in **C 2** (d(C2-O) = 2,623 Å and d (C3-C1) = 2,461 Å) are that the values of the disynaptic basins V(C1,N) and V'(C1,N) were reduced to a population of 2.23

and 1.83, respectively, this decrease led to an appearance of two monosynaptic basins on V(N) and V(C1) with a population of 1.33 and 0.83e.

At **C-3** (**TS-Cm**), d (C2-O) = 2,462 Å and d (C3-C1) = 2,177 Å, the decline in disynaptic basins V(C1,N) and V'(C1,N) is continuous up to 1.98 and 1.46e, respectively, and the increase of two monosynaptic basins on V (N) and V(C1) to a population of 2.08 and 0.98e, respectively, and we notice the division of the monosynaptic basins carried by the C1 carbon into two V(C1) and V'(C1) integrating respectively at 0.50 and 0.48e.

At **C-4**, d(C1-C3) = 2.056 Å and d(O-C2) = 2.396 Å, this is the structure just before the formation of the first C-C single bond, a new monosynaptic basin V(C3) appear at the C3 carbon atom of the double bond C2-C3 with an initial population of 0.32e and two monosynaptic basins, V(C1) and V'(C1), integrating 0.41 and 0.66 respectively, are observed, whilst the disynaptic basin V(C2,C3) was significantly depopulated from 3.10 to 2.74, this monosynaptic basin V(C3) can be associated with the pseudoradical carbon center C3 needed for the formation of single C-C bonds via the sharing model [3].

At **C-5**, d(C1-C3) = 1.997 Å and d(O-C1) = 2.356 Å, the two monosynaptic basins V(C1) and V(C3) merged into a new disynaptic basin V(C2, C3), integrating an initial population of 0.73e. This relevant topological change may be associated with the formation of the first single bond C1-C3 at a distance of 1.94 Å.

At **C-8**, d(C1-C3) =1.710 Å and d(O-C2)=2.177 Å, This is the structure just before the formation of the second single CO bond, we observe the appearance of a monosynaptic basin V(C2), integrating 0.18e, and a monosynaptic basin V(O), integrating 0.43e are observed.

At **C-9**,d(C1-C3) = 1.666 Å and d(O-C2) = 2.128 Å, the two monosynaptic basins V(C2) and V(O) present in C-8 have merged into a new disynaptic basin V(C2,O), integrating 0.11e. This topological change is associated with the formation of the second C1-O single bond, which takes place at a C-O distance of 2.074 Å.

We observe the appearance of a monosynaptic basin V(O), in **C-12** (d(C1-C3) = 1.564 Å and d(O-C2) = 1.812 Å,) and **C-13** (d(C1-C3) = 1.564 Å and d(O-C2) = 1.805 Å,) integrating 0.15 and 0.11 e, respectively, are observed, in **C-14** (d(C1-C3) = 1.521 Å and d(O-C2) = 1.492 Å,), a monosynaptic basin V(O), in C-12. The monosynaptic basin V(O) in C-12 and in C-13, has been added to the bisynaptic basin V(O,C2) (1.23e).

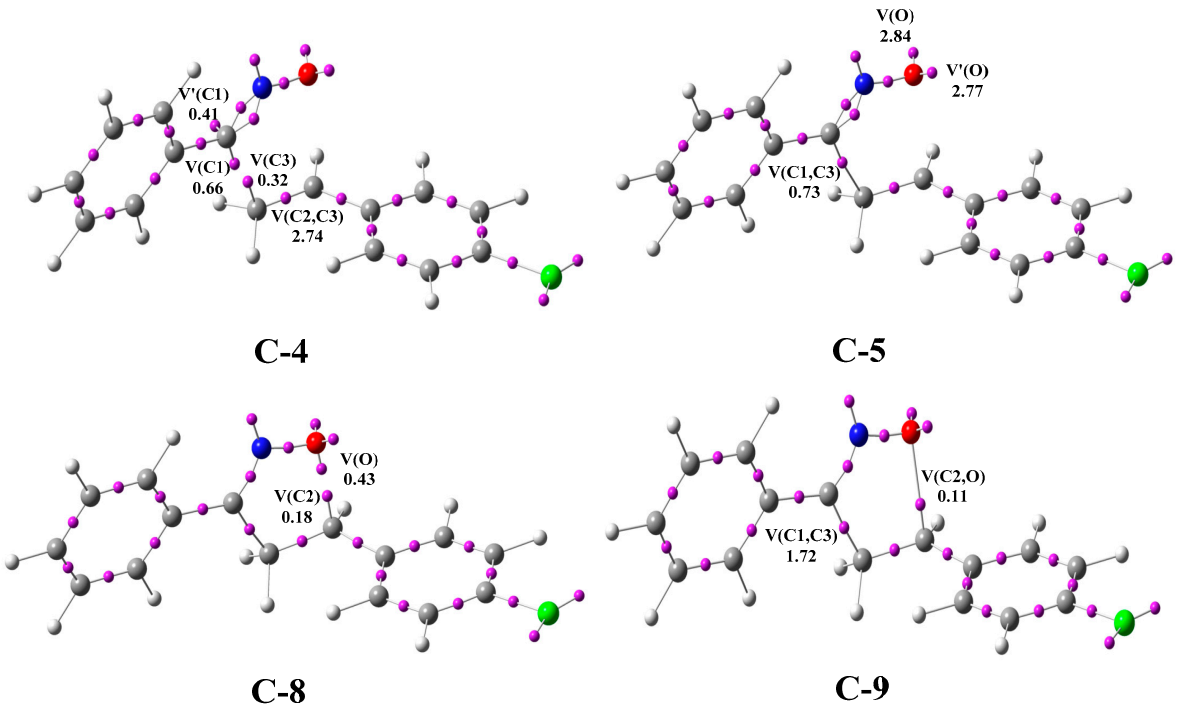


Figure S1. ELF attractor positions for the structures involved in the formation of the C–C and C–O single bonds along the most favorable TS-B-m reaction path associated with the 32CAreaction of 1-chloro-4-vinylbenzene **2** and benzonitrile oxide **3**

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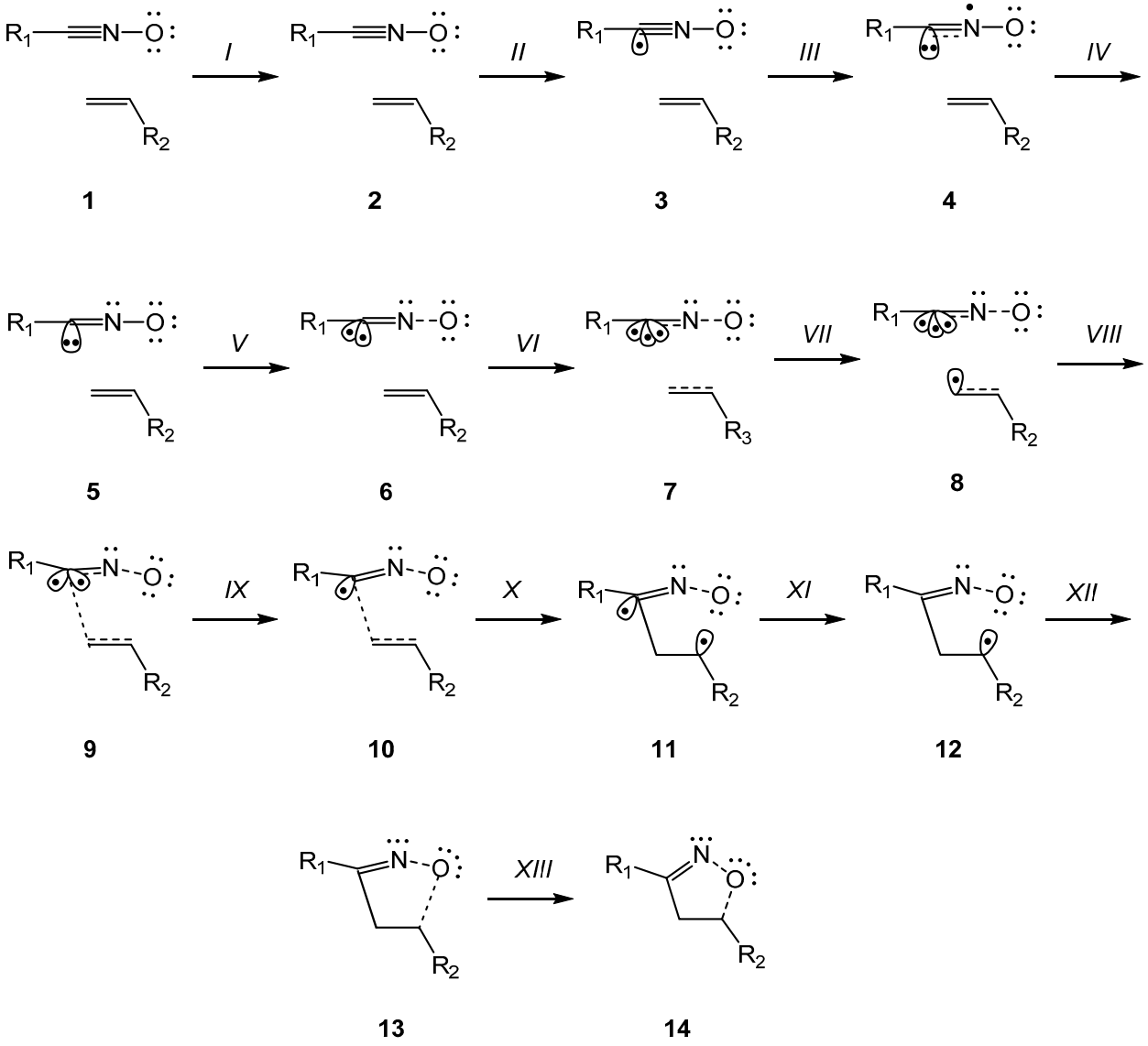
3. L.R. Domingo; A new C–C bond formation model based on the quantum chemicaltopology of electron density, RSC Adv. 4 (2014) 32415-32428.



Scheme S1, Essential the fourteen phases (**1** – **14)** characterizing the molecular mechanism of the 32CA reaction between 1-bromo-4-vinylbenzene **1** and 1-chloro-4-vinylbenzene **2** with benzonitrile oxide **3**

B3LYP/6-311++G(d,p) Cartesian coordinates and electronic energies for TSs structures, together with the single imaginary frequencies

TS-B-m

E(RB3LYP) = -3282.99808619 A.U.
1 imaginary frequencies -408.0822 cm**-1

C	-0.32906700	1.91043900	-0.74806200
O	-1.08473500	1.90623900	1.59274300
C	-2.70421900	0.76834800	0.40835400
C	-1.48726100	1.39734200	-1.28393600
H	-0.27178100	2.97909100	-0.57823500
H	-1.49515600	0.41085000	-1.73303800
H	-2.24073900	2.08726700	-1.64496700
N	-2.08804000	1.25577200	1.33329700
C	-3.86702500	-0.05919200	0.18556400
C	-4.42089000	-0.19528700	-1.09587100
C	-4.45988400	-0.74632700	1.26252600
C	-5.54178200	-0.99635800	-1.29543900
H	-3.97852500	0.32916600	-1.93278700
C	-5.58057200	-1.53882700	1.05305300
H	-4.03407800	-0.64683300	2.25337400
C	-6.12636800	-1.66948100	-0.22526600
H	-5.95978100	-1.09091800	-2.29108800
H	-6.02910600	-2.05970600	1.89140700
H	-6.99960200	-2.29151900	-0.38361100
C	0.91471200	1.17198400	-0.52643500
C	1.01097500	-0.22429300	-0.65057200
C	2.07846200	1.87870400	-0.18245400
C	2.21557200	-0.88683300	-0.44900000
H	0.13413900	-0.81100700	-0.89768900
C	3.29247600	1.23170000	0.01898200
H	2.02991700	2.95612000	-0.06715700
C	3.35155200	-0.15149600	-0.11802500
H	2.27091400	-1.96356800	-0.54518000
H	4.17830100	1.79536400	0.28162000
Br	5.01741700	-1.05934700	0.15576600

TS-B-m THF

E(RB3LYP) = -3283.00675874 A.U.
1 imaginary frequencies -428.9515 cm**-1

C	-0.34046000	1.93370000	-0.70799800
O	-1.09525300	1.90422800	1.67471900
C	-2.70813400	0.78554500	0.45450600
C	-1.50748300	1.42814200	-1.23011900
H	-0.27539500	3.00145200	-0.53444000

H	-1.52878600	0.44288500	-1.68145000
H	-2.26143000	2.12558700	-1.57519400
N	-2.10545000	1.25623200	1.39468600
C	-3.85287500	-0.05837500	0.19359900
C	-4.46975000	-0.06973200	-1.06621800
C	-4.35739400	-0.88672800	1.21473000
C	-5.57189700	-0.88862300	-1.29799700
H	-4.09387100	0.56178100	-1.86034400
C	-5.46110500	-1.69555400	0.97378600
H	-3.88043900	-0.88518500	2.18706500
C	-6.07183900	-1.70177300	-0.28223200
H	-6.04119600	-0.88746000	-2.27484400
H	-5.84357900	-2.32625300	1.76801500
H	-6.93024600	-2.33719000	-0.46617700
C	0.90263800	1.18818200	-0.50457000
C	0.98619800	-0.21059400	-0.62042400
C	2.07751600	1.89175300	-0.18898400
C	2.19051500	-0.87991000	-0.43514400
H	0.10261100	-0.79398900	-0.84962300
C	3.29167800	1.23798800	-0.00444300
H	2.04063300	2.97091500	-0.08742200
C	3.33570300	-0.14697000	-0.13038800
H	2.23444700	-1.95765800	-0.52508800
H	4.18499800	1.80027700	0.23455600
Br	5.00378700	-1.06585500	0.12273600

TS-B-o

E(RB3LYP) = -3282.99271118 A.U.
1 imaginary frequencies -442.3900 cm**-1

C	-1.57540300	-3.15589600	0.78341400
O	-2.76355800	-3.01054100	-0.99931800
C	-2.58139000	-0.81329000	-0.39978800
C	-1.24583600	-1.84235900	1.06243800
H	-2.40323400	-3.62921800	1.29293700
H	-0.88396200	-3.81778600	0.28002000
H	-1.77224400	-1.35874500	1.87981400
N	-2.93431600	-1.78135500	-1.04434700
C	0.06885000	-1.25204900	0.72295000
C	0.61551300	-0.25102700	1.53751300
C	0.80571300	-1.65838600	-0.40077400
C	1.85672900	0.31788000	1.26026500
H	0.06611300	0.08644600	2.40999300
C	2.04611900	-1.10041300	-0.69190500
H	0.40056600	-2.40974900	-1.06922700
C	2.56437900	-0.11409400	0.14441200
H	2.26474600	1.08515200	1.90578900
H	2.59988700	-1.42436200	-1.56388200
C	-2.78422200	0.61081500	-0.27721500
C	-1.74881900	1.50837900	-0.58297200
C	-4.01380000	1.10734200	0.18958400
C	-1.94993300	2.87773200	-0.44014900

H	-0.79962900	1.12751700	-0.93707800
C	-4.20662800	2.47735500	0.32415300
H	-4.80965500	0.41356500	0.43265000
C	-3.17584800	3.36459900	0.01158300
H	-1.14889300	3.56524100	-0.68597000
H	-5.16136300	2.85371200	0.67322900
H	-3.32896400	4.43240400	0.11911500
Br	4.27350700	0.66200400	-0.25409900

TS-B-o THF

E(RB3LYP) = -3283.00085667 A.U.
1 imaginary frequencies -448.8600 cm**-1

C	-1.78182000	-3.15458200	0.72000200
O	-2.99764900	-2.85286000	-1.08584700
C	-2.69673200	-0.71251000	-0.32988500
C	-1.39759500	-1.87063300	1.05121300
H	-2.63024600	-3.61031500	1.21151900
H	-1.13195300	-3.81906300	0.16705400
H	-1.89448400	-1.40821000	1.89843700
N	-3.11083600	-1.61203300	-1.03315300
C	-0.06881500	-1.30706300	0.71328500
C	0.49671700	-0.32313200	1.53641800
C	0.65956700	-1.72168800	-0.41263200
C	1.75109600	0.22045800	1.26555900
H	-0.04515900	0.02023200	2.41089400
C	1.91380800	-1.19051500	-0.69781600
H	0.24473500	-2.46257800	-1.08632700
C	2.44923600	-0.22260500	0.14815600
H	2.17206100	0.97473700	1.91788000
H	2.46048800	-1.52306400	-1.57089600
C	-2.67112000	0.72632300	-0.22402200
C	-3.05691600	1.35383700	0.97101500
C	-2.23034900	1.50710200	-1.30691400
C	-3.01897400	2.74074000	1.07311100
H	-3.39104400	0.75426000	1.80909500
C	-2.20249600	2.89329500	-1.19716400
H	-1.92058700	1.02219000	-2.22443700
C	-2.59407000	3.51248200	-0.00904300
H	-3.32397400	3.21939900	1.99624700
H	-1.87022700	3.49065700	-2.03818200
H	-2.56627100	4.59281600	0.07352300
Br	4.18127100	0.51848500	-0.24153300

TS-C-m

E(RB3LYP) = -1169.07833287A.U.
1 imaginary frequencies -408.6532cm**-1

C	-0.50333100	1.70674200	-0.79151600

O	0.27172400	1.85700800	1.53964600
C	1.96275500	0.79904200	0.38174000
C	0.68804600	1.26771600	-1.32025900
H	-0.64499200	2.77318000	-0.66215200
H	1.38059600	2.00153300	-1.71510100
H	0.77210700	0.26843700	-1.73177400
N	1.31950200	1.27438700	1.29445500
C	3.17737600	0.04446400	0.17670600
C	3.74647300	-0.07288000	-1.09997300
C	3.80483700	-0.59134600	1.26541700
C	4.91601700	-0.80523300	-1.28340400
H	3.27761200	0.41285900	-1.94586300
C	4.97388500	-1.31523900	1.07204700
H	3.36732600	-0.50662600	2.25253300
C	5.53444500	-1.42768100	-0.20157600
H	5.34526600	-0.88587900	-2.27548300
H	5.44864000	-1.79713100	1.91923700
H	6.44527300	-1.99663300	-0.34733000
C	-1.68121400	0.88009700	-0.52580800
C	-1.66500000	-0.52336400	-0.59475500
C	-2.89439900	1.50353000	-0.19119900
C	-2.80860600	-1.27216100	-0.34854600
H	-0.74631600	-1.04626800	-0.83232800
C	-4.04840600	0.76877000	0.05385100
H	-2.93168800	2.58497100	-0.11770100
C	-3.99631700	-0.61883800	-0.02818700
H	-2.78212600	-2.35321700	-0.40067800
H	-4.97628200	1.26441300	0.30920700
Cl	-5.44735800	-1.56224300	0.28128600

TS-C-m THF

E(RB3LYP) = -1169.08694233 A.U.

1 imaginary frequencies -428.6248 cm**-1

C	-0.49588400	1.71143800	-0.76569500
O	0.27952400	1.84127500	1.60563200
C	1.96676800	0.80104600	0.41651900
C	0.70119200	1.27444000	-1.28115800
H	-0.64058500	2.77778800	-0.63736600
H	1.39590600	2.01175400	-1.66535700
H	0.79388600	0.27473500	-1.68965900
N	1.33567500	1.26371100	1.34175700
C	3.17566700	0.04353300	0.18054400
C	3.76774900	0.00342000	-1.09047900
C	3.77027100	-0.66983300	1.23949600
C	4.93298400	-0.73070500	-1.29679900
H	3.32371500	0.54720800	-1.91371800
C	4.93583200	-1.39442100	1.02331200
H	3.31366200	-0.64595600	2.22124600
C	5.52127800	-1.42978200	-0.24423700
H	5.38169900	-0.75269300	-2.28302100

H	5.38678100	-1.93684500	1.84631400
H	6.42833800	-1.99963400	-0.40841400
C	-1.67671500	0.88371300	-0.51410400
C	-1.65426100	-0.52126100	-0.56836000
C	-2.89845100	1.50929800	-0.21187200
C	-2.80116500	-1.27077800	-0.33587500
H	-0.73131600	-1.04525700	-0.78505100
C	-4.05611900	0.77379500	0.01900800
H	-2.94298800	2.59151600	-0.15737000
C	-3.99508200	-0.61436100	-0.04577300
H	-2.76846500	-2.35207400	-0.37709000
H	-4.98955100	1.27204000	0.24757300
Cl	-5.45302200	-1.56094200	0.24808300

TS-C-o

E(RB3LYP) = -1169.07277200 A.U.
1 imaginary frequencies -443.7021 cm**-1

C	-0.72346500	3.19276300	0.76523700
O	-1.93773200	3.12264100	-1.02275700
C	-1.98465900	0.94386500	-0.33913100
C	-0.52492800	1.85776800	1.06238500
H	0.01866000	3.77242100	0.23389200
H	-1.49290800	3.75565100	1.27543100
H	-1.07584100	1.44587500	1.90260400
N	-2.24087000	1.91890500	-1.01779500
C	0.70379900	1.11852000	0.69175800
C	1.13872200	0.04597600	1.48191000
C	1.46337600	1.44800400	-0.44163500
C	2.29561400	-0.66462300	1.17319900
H	0.56794800	-0.23605100	2.36025500
C	2.62216400	0.74942000	-0.76241000
H	1.14152500	2.25258500	-1.09318900
C	3.03140400	-0.30408500	0.05072200
H	2.62179200	-1.48703600	1.79720100
H	3.19967900	1.01396300	-1.63925300
C	-2.20302500	-0.48026500	-0.25038500
C	-2.98888500	-1.00953500	0.78553500
C	-1.59420300	-1.35154000	-1.16815700
C	-3.17869500	-2.38343300	0.88651500
H	-3.45499200	-0.33832600	1.49732300
C	-1.79243600	-2.72403100	-1.06248100
H	-0.97480500	-0.94417300	-1.95753700
C	-2.58236500	-3.24259200	-0.03672200
H	-3.79482000	-2.78408400	1.68325500
H	-1.32549300	-3.38994800	-1.77895200
H	-2.73182700	-4.31321800	0.04410900
Cl	4.49379600	-1.19637500	-0.35509200

TS-C-o THF

E(RB3LYP) = -1169.08105997 A.U.
1 imaginary frequencies-449.9174 cm**-1

C	-0.76013800	3.19693600	0.76354800
O	-2.05619900	3.09783600	-1.00753400
C	-2.02162200	0.92146800	-0.29785200
C	-0.54275700	1.86666200	1.06198800
H	-0.04248700	3.77978900	0.20232500
H	-1.52570400	3.75201700	1.28784400
H	-1.07435900	1.45700400	1.91529400
N	-2.33200500	1.88163100	-0.97393900
C	0.68840700	1.13668600	0.67650300
C	1.14065900	0.07344200	1.47066000
C	1.43314300	1.46763900	-0.46636000
C	2.30198400	-0.62842900	1.15523500
H	0.58227600	-0.20863100	2.35649700
C	2.59562400	0.77786300	-0.79539700
H	1.10159300	2.26655300	-1.11953400
C	3.02054100	-0.26554700	0.02240100
H	2.64044800	-1.44297600	1.78293700
H	3.15965600	1.04383200	-1.68041600
C	-2.18474500	-0.50970200	-0.21052600
C	-2.69483600	-1.09276700	0.96027300
C	-1.80367000	-1.33080000	-1.28592000
C	-2.83848700	-2.47398900	1.04452800
H	-2.98370500	-0.46235000	1.79255000
C	-1.95654700	-2.71025900	-1.19415300
H	-1.39855100	-0.88139400	-2.18417300
C	-2.47159800	-3.28427400	-0.03082100
H	-3.23950500	-2.91780700	1.94815200
H	-1.66933000	-3.33803400	-2.02958200
H	-2.58485200	-4.36000000	0.03793000
Cl	4.49249400	-1.14774600	-0.39274200