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# AZIRINO[*c*]IMIDAZOLYL YLIDES IN THE DOMINO REACTION OF 2,2-DIALKYL-4,6-DIARYL-1,3-DIAZABICYCLO[3.1.0]HEX-3-ENES WITH DICHLOROCARBENES. SYNTHESIS OF (1*RS*,5*SR*,6*RS*)-4-(ALK-1-ENYL)-1,5-DIARYL-3,7,7-TRICHLORO-2,4-DIAZABICYCLO[4.1.0]HEPT-2-ENES*

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*The reaction of 2,2-dialkyl-4,6-diaryl-1,3-diazabicyclo[3.1.0]hex-3-enes with dichlorocarbene to give (1RS,5SR,6RS)-4-(alk-1-enyl)-1,5-diaryl-3,7,7-trichloro-2,4-diazabicyclo[4.1.0]hept-2-enes has been studied. Quantum-chemical calculations using the DFT B3LYP/6-31G(d) method have confirmed that the mechanism of the reaction includes the formation of azirino[c]imidazolium ylides and coordinated opening of the imidazole and aziridine rings with subsequent cyclization and dichloropropane formation.*

**Keywords:** aziridines, carbenes, imidazoles, iminium ylides, pyrimidines, cascade reactions, domino reactions.

Domino reactions with the participation of several intermediates allows a considerable increase in molecular complexity in a single synthetic stage. Intensive investigations of such reactions have been carried out in recent years since they permit a reduction in the expenditure of energy and labor, reagents and additional materials and they lessen the contamination of the environment through the absence of separation of unnecessary intermediate products [1-6]. In particular great attention has been placed on domino processes involving carbenes (carbenoids) and nitrogen or oxygen ylides [7-11]. The greatest amount of work in this regard is concerned with a study of reactions in which the reaction sequence begins with generation of a carbenoid from a diazo compound [12-17]. Cascade carbene-ylide transformations involving other carbenes have also been studied for dichloro- [12, 18, 19], monofluoro- [20, 21], and difluorocarbenes [12, 22-28]. The reaction of carbenes and carbenoids with azirines leading to the formation of azirinyl ylides is an example of carbene-ylide reactions involving a three-membered ring. The strain energy of such a ring governs the

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* Dedicated to the respected memory of A. A. Potekhin

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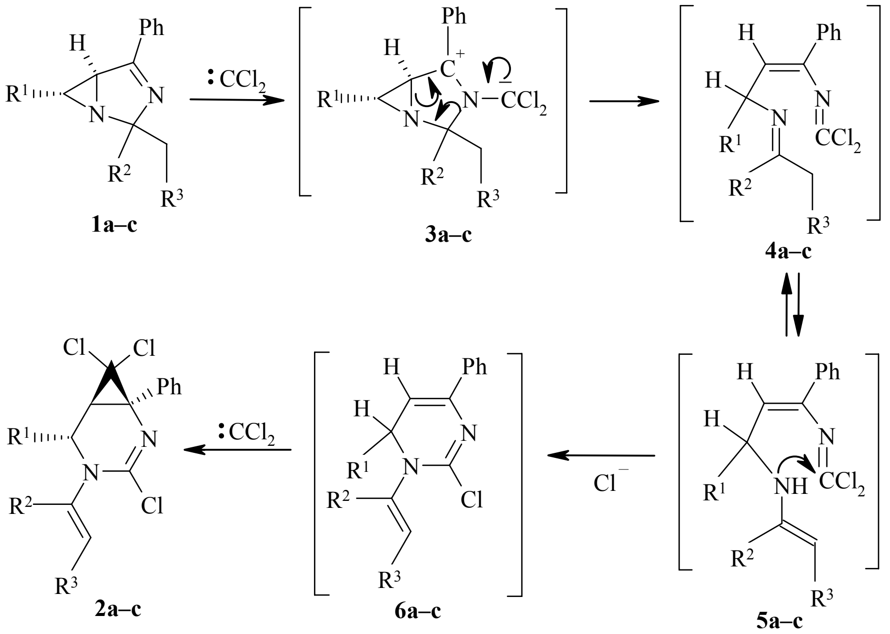
occurrence of unusual reactions atypical of other iminium ylides [29-32]. Reactions in which growth of a domino process would be achieved by opening a strained three-membered ring not included in the composition of the ylide system but as a substituent in the ylide are unknown. In this report we have carried out the first example of such a reaction.

The 1,3-diazabicyclo[3.1.0]hex-3-ene system, containing an amine or imine nitrogen atom in its composition, can react with an electrophilic carbene to give either ammonium or iminium ylides. In the latter case the ylide intermediate acts as a 1,3-dipole containing a strained aziridine ring as substituent at an ylide carbon atom. For generation of such ylides as the carbene component of the reaction we have chosen dichlorocarbene as the most synthetically versatile and available of functionally-substituted carbenes and the 2,2-dialkyl-4,6-diaryl-1,3-diazabicyclo[3.1.0]hex-3-enes **1a-c** as the compounds containing the 1,3-diazabicyclo[3.1.0]hex-3-ene system. The dichlorocarbene was generated by basic hydrolysis of chloroform under phase transfer catalytic conditions ($CHCl_3$ /KOH / $BnEt_3NCl$). The diazabicyclohexenes **1a-c** which show interest as photochromic compounds can be readily prepared from the corresponding chalcone dibromide and ketone $R^2C(O)CH_2R^3$ in the presence of ammonia [33, 34].

The reaction of compounds **1a-c** with dichlorocarbene gave the (1*RS*,5*SR*,6*RS*)-4-(alk-1-enyl)-1,5-diaryl-3,7,7-trichloro-2,4-diazabicyclo[4.1.0]hept-2-enes **2a-c**. The structure of compounds **2a-c** was confirmed from $^1H$ and $^{13}C$ NMR spectroscopy, IR, and elemental analytical data (see Experimental) and the structure of compound **2a** by the X-ray structural method (Fig. 1, Tables 1 and 2).



**a** $R^1$ = 4-$BrC_6H_4$, $R^2$ = Me, $R^3$ = H; **b** $R^1$ = 4-$O_2NC_6H_4$, $R^2$ = Me, $R^3$ = H;
**c** $R^1$ = 4- $O_2NC_6H_4$, $R^2 + R^3 = (CH_2)_4$

The formation of compounds **2a-c** evidently occurs as the result of achieving the following sequence of reactions: the reaction of dichlorocarbene with the unshared electron pair of the imine nitrogen atom of molecules **1a-c** to form the iminium ylides **3a-c** which undergo fission at the C(2)–N(3) bond with simultaneous opening of the three-membered ring at the C(5)–N(1) bond to give the diazatrienes **4a-c**. Tautomerization of imine **4a-c** to enamine **5a-c** in basic medium and subsequent cyclization involving the highly reactive imidoyl chloride group gives the dihydropyrimidines **6a-c**. Compounds **6a-c** contains an "enamine" C=C bond which is potentially highly active with respect to the electrophilic dichlorocarbene. In fact the final reaction products

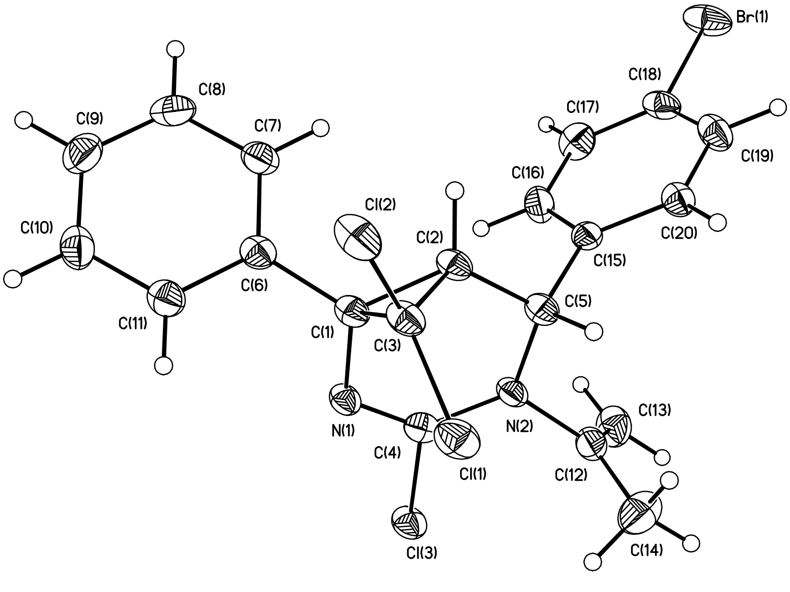


Fig. 1. Molecular structure of compound **2a.**

**2a-c** contain a cyclopropane ring which is formed as the result of addition of the dichlorocarbene to the endocyclic C=C bond of the dihydropyrimidines **6a-c**. At the same time the products of cyclopropane ring formation at the exocyclic C=C double bond of both compounds **2a-c** and **6a-c** are not observed. The reason for the low activity of the C=C bond in compounds **2a-c** towards the dichlorocarbene is likely its shielding by the 5-aryl group on one side and the chlorine atom on the other and this is clearly seen in the steric model of compound **2a** revealed from X-ray structural analysis. Evidently similar shielding of the exocyclic C=C bond hindering the cyclopropane ring formation is also seen in compounds **6a-c**.

It is known that dichloroiminium ylides formed by reaction of dichlorocarbene and N-alkyl-N-arylideneamines with tertiary and secondary alkyl substituents readily undergo 1,3-cyclization to give *gem*-dichloroaziridines [12]. Neither the corresponding *gem*-dichloroaziridines nor any kind of products of their conversion in the reaction of compounds **1a-c** with dichlorocarbene were observed. We have used quantum chemical calculations of the possible routes of stabilization of the model ylide **7** to explain the reason for the absence of the 1,3-cyclization products of the ylides **3a-c** and to understand the mechanism of the reaction of these 1,3-dipoles.

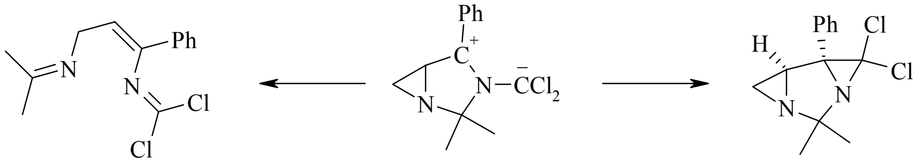
TABLE 1. Basic Bond Lengths ($l$) in the Molecule **2a**

| Bond | $l$, Å | Bond | $l$, Å | Bond | $l$, Å |
|---|---|---|---|---|---|
| Br(1)–C(18) | 1.900(3) | C(1)–C(2) | 1.516(4) | C(10)–C(11) | 1.393(4) |
| Cl(1)–C(3) | 1.747(3) | C(1)–C(3) | 1.519(4) | C(12)–C(13) | 1.354(5) |
| Cl(2)–C(3) | 1.761(3) | C(2)–C(3) | 1.502(4) | C(12)–C(14) | 1.448(5) |
| Cl(3)–C(4) | 1.745(3) | C(2)–C(5) | 1.521(4) | C(15)–C(20) | 1.385(4) |
| N(1)–C(4) | 1.272(4) | C(5)–C(15) | 1.509(4) | C(15)–C(16) | 1.387(4) |
| N(1)–C(1) | 1.448(3) | C(6)–C(11) | 1.390(4) | C(16)–C(17) | 1.382(5) |
| N(2)–C(4) | 1.362(4) | C(6)–C(7) | 1.392(4) | C(17)–C(18) | 1.384(5) |
| N(2)–C(12) | 1.454(4) | C(7)–C(8) | 1.386(4) | C(18)–C(19) | 1.379(4) |
| N(2)–C(5) | 1.480(3) | C(8)–C(9) | 1.379(5) | C(19)–C(20) | 1.381(5) |
| C(1)–C(6) | 1.502(4) | C(9)–C(10) | 1.389(5) | | |

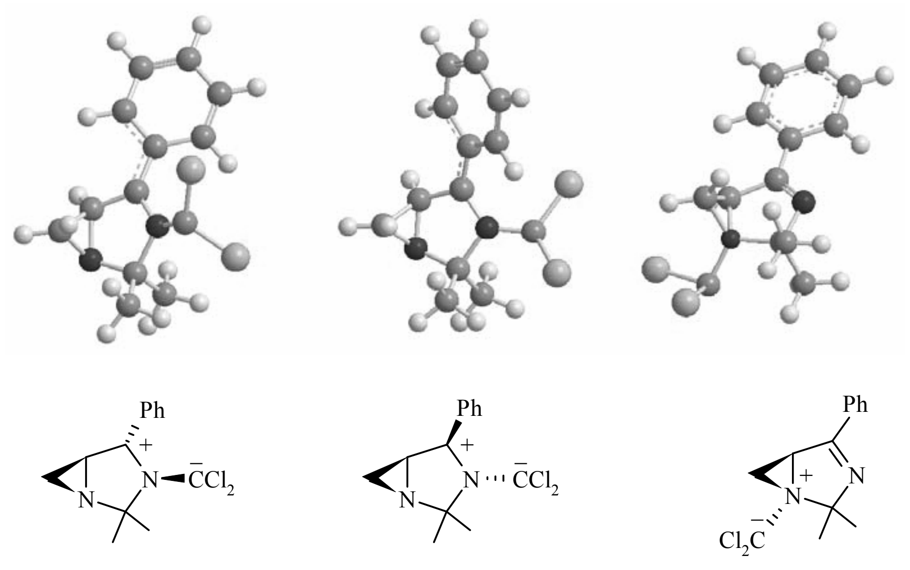
TABLE 2. Basic Valence Angles (ω) in the Molecule **2a**

| Angle | ω, deg | Angle | ω, deg | Angle | ω, deg |
|---|---|---|---|---|---|
| C(4)–N(1)–C(1) | 116.7(2) | C(2)–C(3)–Cl(2) | 116.5(2) | C(6)–C(11)–C(10) | 120.1(3) |
| C(4)–N(2)–C(12) | 122.8(2) | C(1)–C(3)–Cl(2) | 118.1(2) | C(13)–C(12)–C(14) | 125.4(3) |
| C(4)–N(2)–C(5) | 121.2(2) | Cl(1)–C(3)–Cl(2) | 112.19(16) | C(13)–C(12)–N(2) | 119.2(3) |
| C(12)–N(2)–C(5) | 113.5(2) | N(1)–C(4)–N(2) | 130.8(2) | C(14)–C(12)–N(2) | 115.4(3) |
| N(1)–C(1)–C(6) | 110.9(2) | N(1)–C(4)–Cl(3) | 115.9(2) | C(20)–C(15)–C(16) | 118.7(3) |
| N(1)–C(1)–C(2) | 119.1(2) | N(2)–C(4)–Cl(3) | 113.2(2) | C(20)–C(15)–C(5) | 120.1(3) |
| C(6)–C(1)–C(2) | 123.1(2) | N(2)–C(5)–C(15) | 110.8(2) | C(16)–C(15)–C(5) | 121.2(3) |
| N(1)–C(1)–C(3) | 116.5(2) | N(2)–C(5)–C(2) | 111.9(2) | C(17)–C(16)–C(15) | 121.0(3) |
| C(6)–C(1)–C(3) | 119.0(2) | C(15)–C(5)–C(2) | 110.2(2) | C(16)–C(17)–C(18) | 119.1(3) |
| C(2)–C(1)–C(3) | 59.34(19) | C(11)–C(6)–C(7) | 119.8(3) | C(19)–C(18)–C(17) | 120.9(3) |
| C(3)–C(2)–C(1) | 60.44(19) | C(11)–C(6)–C(1) | 118.1(3) | C(19)–C(18)–Br(1) | 119.8(2) |
| C(3)–C(2)–C(5) | 120.4(2) | C(7)–C(6)–C(1) | 122.1(3) | C(17)–C(18)–Br(1) | 119.4(3) |
| C(1)–C(2)–C(5) | 119.8(2) | C(8)–C(7)–C(6) | 119.7(3) | C(18)–C(19)–C(20) | 119.2(3) |
| C(2)–C(3)–C(1) | 60.22(19) | C(9)–C(8)–C(7) | 120.8(3) | C(19)–C(20)–C(15) | 121.1(3) |
| C(2)–C(3)–Cl(1) | 120.3(2) | C(8)–C(9)–C(10) | 119.8(3) | | |
| C(1)–C(3)–Cl(1) | 120.5(2) | C(9)–C(10)–C(11) | 119.8(3) | | |

The removal of the 6-aryl group from ylide **3** on going to ylide **7** for simplifying the calculation seems justified since the aryl substituent at C-6 in 2,2-dialkyl-4,6-diaryl-1,3-diazabicyclo[3.1.0]hex-3-enes does not prove to affect either the cyclization or the fission of ylide **3**. Using the DFT B3LYP/6-31G(d) method and GAUSSIAN 03 program package we have carried out a full optimization of the geometry of ylide **7**, its



**9** **7** **8**



**7a** **7b** **10**

Fig. 2. Optimized structures of the ylides **7a,b** and **10.**

precursor (2,2-dimethyl-4-phenyl-1,3-diazabicyclo[3.1.0]hex-3-ene) (**1d**), diazatricycloheptane **8** formed on cyclization of ylide **7**, triene **9** formed by fission of ylide **7**, the transition states for the reactions **7** → **8**, **7** → **9**, and the aziridinium ylide **10** (Figures 2 and 3). As seen in the data in Table 3 the calculation reproduces well the geometry of the 1,3-diazabicyclo[3.1.0]hex-3-ene system which is an indirect confirmation of the correctness of using the simplified structure in the calculation.

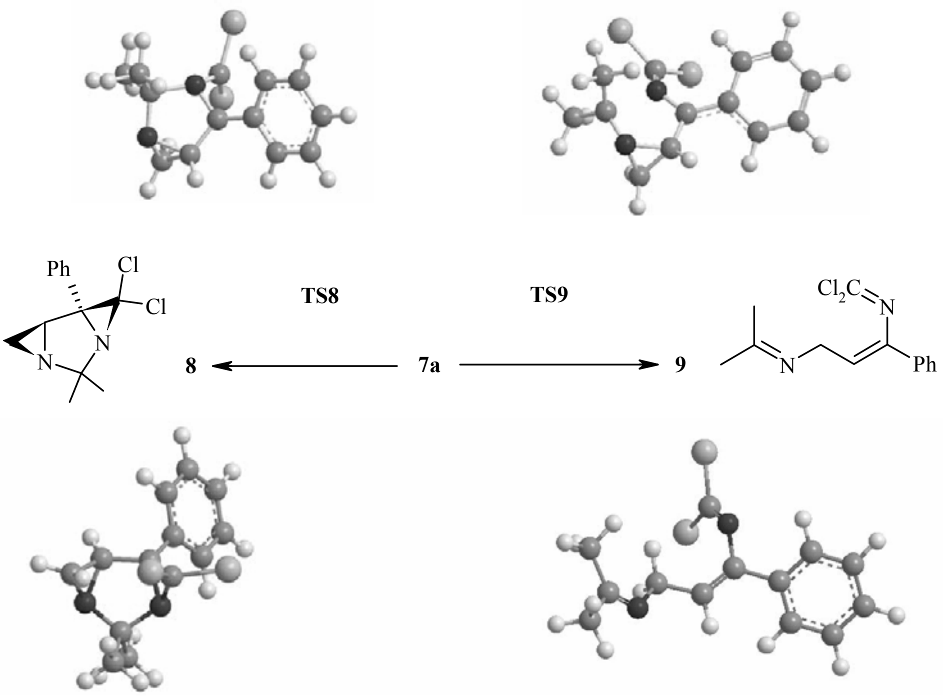


Fig. 3. Optimized structures for the diazatricycloheptane **8**, triene **9**, and transition states **TS8** and **TS9** for cyclization and fission of ylide **7a**.

Two stationary points were found as the result of the calculations of ylide **7** which correspond to the two conformations of ylide **7a,b**. The conformation of iminium ylide **7a** is 7.9 kcal/mol more stable than conformation **7b**. The aziridine ylide **10**, which can be formed by treatment of the electrophilic dichlorocarbene with the unshared nitrogen pair of the aziridine ring of 1,3-diazabicyclo[3.1.0]hex-3-ene is even less stable, its energy being greater than that of ylide **7a** by 9.1 kcal/mol.

TABLE 3. Bond lengths (*l*) and Valence Angles (ω) in the 1,3-Diazabicyclo[3.1.0]hex-3-ene Systems of Molecule 1d (Calculated Data) and 1b (X-ray Analytical Data [34]).

| Bond | *l*, Å | | Angle | ω, deg. | |
|---|---|---|---|---|---|
| | **1d** | **1b** | | **1d** | **1b** |
| N(1)–C(2) | 1.506 | 1.508(4) | N(1)–C(2)–N(3) | 107.9 | 107.8(2) |
| C(2)–N(3) | 1.476 | 1.475(4) | C(2)–N(3)–C(4) | 108.8 | 108.9(2) |
| N(3)–C(4) | 1.285 | 1.280(3) | N(3)–C(4)–C(5) | 113.0 | 113.2(2) |
| C(4)–C(5) | 1.505 | 1.499(4) | C(4)–C(5)–N(1) | 105.3 | 105.5(2) |
| N(1)–C(5) | 1.473 | 1.474(3) | C(2)–N(1)–C(5) | 104.5 | 104.1(2) |
| N(1)–C(6) | 1.465 | 1.470(4) | N(1)–C(6)–C(5) | 59.7 | 59.2(2) |
| C(5)–C(6) | 1.494 | 1.502(4) | C(5)–N(1)–C(6) | 61.1 | 61.3(2) |

Hence the investigated reaction sequence can only be realized *via* ylide **7a** for which further calculations were carried out.

The ylide **7a** can be cyclized to give the *gem*-dichloroaziridine **8**, *cis*-orientated with respect to the three-membered ring already existing in the starting molecule, or undergo fission to triene **9** *via* the transition states **TS(8)** and **TS(9)** respectively.

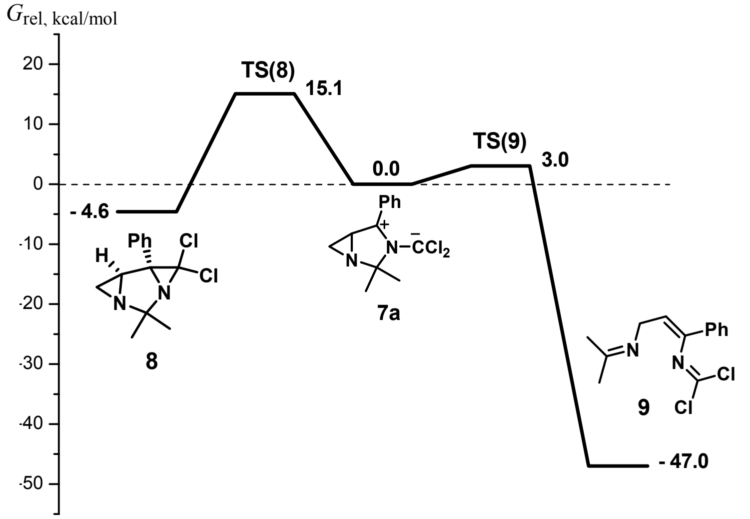


Fig. 4. Energy diagram for the reactions of ylide **7a.**

As is evident from the results of the calculations represented in Figure 4 the barrier to activation of fission of ylide **7** to triene **9** is significantly lower than the barrier to cyclization of the same ylide to aziridine **8**. This is evidently the reason that neither the corresponding *gem*-dichloroaziridines nor any of their reaction products were found when reacting compounds **1a-c** with dichlorocarbene.

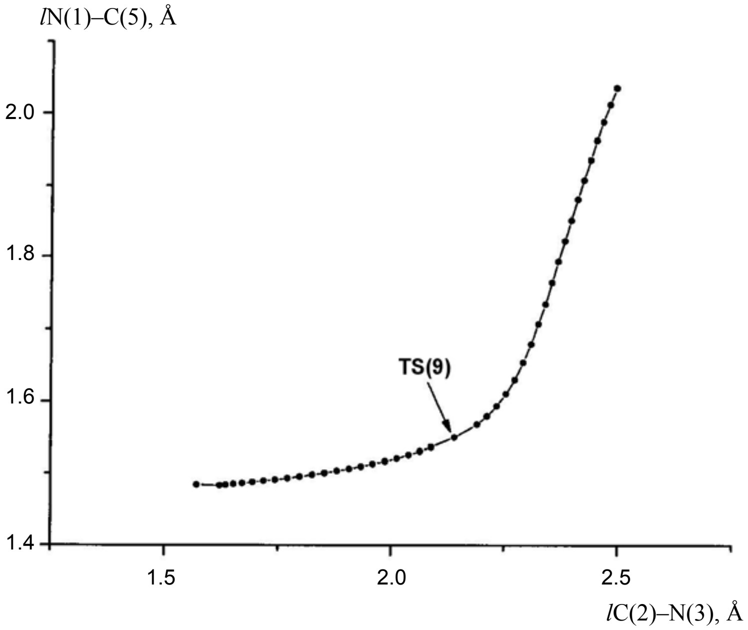


Fig. 5. Change in interatomic distances in the five-membered ring [C(2)–N(3)] and three-membered ring [C(5)–N(1)] for movement along the reaction coordinate **7** → **9**.

Analysis of the change in distances between the C(2)–N(3) and C(5)–N(1) atoms with movement along the reaction coordinates **7** → **9** (Fig. 5) shows that the cleavage of the bond in the five membered ring [C(2)–N(3)] and three membered ring [C(5)–N(1)] occur together but are not synchronized.

Hence the reaction of the diazabicyclohexenes **1a-c** with dichlorocarbene (generated using base under phase-transfer catalytic conditions) occurs involving two molecules of the carbene to give the 2,4-diazabicyclo[4.1.0]hept-2-enes **2a-c**. Attack of the dichlorocarbene occurs at the imine nitrogen atom of the substrate to form the azirino[*c*]imidazolium ylides **3a-c**. Data for the possible means of stabilizing the *gem*-dichloro-substituted ylide intermediate **7** calculated by the DFT B3LYP/6-31G(d) method fully agree with the experimental data and point to the important role of the three-membered ring in the aziridine-substituted 1,3-dipole. The presence of this strained element in the structure makes possible the occurrence in the intermediates **3a-c** of a clevage of the C–N bond, uncharacteristic of iminium ylides, which happens with an extremely low activation barrier simultaneously with opening of the aziridine ring. This is the reason that the 1,3-diazabicyclo[3.1.0]hexenes do not form the expected *gem*-dichloroaziridines under conditions of dichlorocarbene formation but, as a result of a cascade process including formation of an iminium ylide, opening two rings with recyclization and cyclopropane formation to lead to a cyclopropanopyrimidine derivatives.

## EXPERIMENTAL

IR spectra for compound **1a** were recorded on a Thermo Nicolet Avatar 370 FT-IR instrument (attenuated total reflection technique) and for compounds **1b,c** on a Specord M80 instrument for KBr tablets. The $^1$H and $^{13}$C NMR spectra were taken on a Bruker DPX-300 instrument (300 and 75 MHz respectively) using $CDCl_3$ and using the solvent signals at δ 7.26 ($^1$H) and 77.0 ppm ($^{13}$C) as internal standards. X-ray analysis was performed on an STOE IPDS II diffractometer. Elemental analysis was obtained on a EuroEA3000 CHN-analyzer. Merck 60 silica gel was used to separate the reaction mixtures.

**Compounds 1a,b** were prepared by the method reported in [34] and compound **1c** by that in [33].

Quantum-chemical calculations were made using the Gaussian 03 program package [35]. The hybrid function B3LYP [36, 37] and 6-31G(d) base set [38] were used for optimization of all of the stationary points in the gas phase. Frequency analysis was used to assign the stationary points to minima or first order saddle points. All of the transition states were associated with only one imaginary frequency and their links to the starting compounds and products were tested using the IRC procedure [35]].

**Synthesis of (1*RS*,5*SR*,6*RS*)-5-(4-Bromophenyl)-3,7,7-trichloro-4-isopropenyl-1-phenyl-2,4-diazabicyclo[4.1.0]hept-2-ene (2a) (General Method)**. Finely divided KOH (1.1 g, 20 mmol) was added with vigorous stirring over 3 h to a solution of the diazabicyclohexene **1a** (0.818 g, 2.40 mmol) and benzyltriethylammonium chloride (0.05 g, 0.22 mmol) in chloroform (10 ml) freed from stabilizer and the reaction mixture temperature was maintained at 20-22ºC by means of a water bath. The reaction mixture was filtered through an $Al_2O_3$ layer (1 cm), the filtrate was evaporated *in vacuo*, and column chromatography of the residue (silica gel, hexane–ethyl acetate eluent) gave compound **2a** (0.164 g, 15%) with mp 162-164ºC (decomp., mixture of ether and hexane). IR spectrum (attenuated total reflection), ν, cm$^{-1}$: 1617 (C=N). $^1$H NMR spectrum ($CDCl_3$), δ, ppm: 7.30-7.58 (9H, Ar); 5.02 (1H, s, $C=CH_2$); 4.85 (1H, s, H-5); 4.66 (1H, s, $C=CH_2$); 2.59 (1H, s, H-6); 1.77 (3H, s, $CH_3$). $^{13}$C NMR spectrum ($CDCl_3$), δ, ppm: 145.3 (N=CCl); 143.8 ($\underline{C}=CH_2$); 140.8, 137.4, 132.5, 128.8, 128.5, 128.4, 128.3, 122.6 (Ar); 117.5 ($=CH_2$); 68.6 ($CCl_2$); 59.0 (C-5); 53.3 (C-1); 37.2 (C-6); 21.5 ($CH_3$). Found, %: C 51.12; H 3.58; N 5.71. $C_{20}H_{16}BrCl_3N_2$. Calculated, %: C 51.04; H 3.43; N 5.95.

**(1*RS*,5*SR*,6*RS*)-3,7,7-Trichloro-4-isopropenyl-5-(4-nitrophenyl)-1-phenyl-2,4-diazabicyclo-[4.1.0]hept-2-ene (2b)** was prepared by a similar method from compound **1b** (0.799 g, 2.60 mmol) in 0.232 g (20%) yield with mp 173-175ºC (decomp., EtOH). IR spectrum (KBr), ν, cm$^{-1}$: 1620 (C=N). $^1$H NMR spectrum ($CDCl_3$), δ, ppm: 8.33-8.29 (2H, m, Ar); 7.62-7.58 (2H, m, Ar); 7.43-7.36 (5H, m, $C_6H_5$); 5.03 (1H, s, C=$CH_2$); 5.01 (1H, s, H-5); 4.62 (1H, s, C=$CH_2$); 2.59 (1H, s, H-6); 1.81 (3H, s, $CH_3$). $^{13}$C NMR spectrum ($CDCl_3$), δ, ppm: 148.8, 148.0 (Ar); 145.1 (N=CCl); 143.7 ($\underline{C}$=$CH_2$); 137.0, 128.6, 128.5, 128.2, 128.1, 124.7 (Ar); 117.85 (=$CH_2$); 68.6 ($CCl_2$); 58.7 (C-5); 53.3 (C-1); 37.0 (C-6); 21.4 ($CH_3$). Found, %: C 54.85; H 3.75; N 9.50. $C_{20}H_{16}Cl_3N_3O_2$. Calculated, %: C 55.00; H 3.69; N 9.62.

**(1*RS*,*5SR*,*6RS*)-3,7,7-Trichloro-4-(cyclohex-1-enyl)-5-(4-nitrophenyl)-1-phenyl-2,4-diazabicyclo-[4.1.0]hept-2-ene (2c)** was prepared similarly from compound **1c** (0.410 g, 1.18 mmol) in 0.174 g (31%) yield with mp 167-169ºC (decomp., EtOH). IR spectrum (KBr), ν, cm$^{-1}$: 1620 (C=N). $^1$H NMR spectrum ($CDCl_3$), δ, ppm: 8.33-8.29 (2H, m, Ar); 7.60-7.57 (2H, m, Ar); 7.42-7.37 (5H, m, $C_6H_5$); 5.27 (1H, br. s, C=CH); 4.98 (1H, s, H-5); 2.56 (1H, s, H-6); 1.49-2.01 (8H, m, $CH_2$). $^{13}$C NMR spectrum ($CDCl_3$), δ, ppm: 149.2, 147.9 (Ar); 144.8 (N=CCl); 139.7 ($\underline{C}$=CH; 137.14 ($C_6H_5$); 130.5 (C=$\underline{C}$H); 128.5, 128.4, 128.2, 128.1, 124.5 (Ar); 68.8 ($CCl_2$); 58.9 (C-5); 53.3 (C-1); 36.8 (C-6); 28.3, 24.7, 22.5, 21.1 ($CH_2$). Found, %: C 57.99; H 4.28; N 8.57. $C_{23}H_{20}Cl_3N_3O_2$. Calculated, %: C 57.94; H 4.23; N 8.81.

**X-ray Parameters for Compound 2a**. A single crystal for X-ray structural analysis was grown from a mixture of diethyl ether and hexane. $C_{29}H_{21}NO_2$. $M = 415.47$, $a = 11.9564(13)$, $b = 15.3773(14)$, $c = 12.2068(13)$ Å, $\beta = 119.32(2)^\circ$, $V = 1956.7(3)$ Å$^3$, $Z = 4$, $d = 1.597$ mg/m$^3$, monoclinic crystal system, space group Cc (N 9), radiation source MoKα, $\lambda = 0.7103$ Å, temperature 133(2) $K$, $R_{\text{all}} = 0.0231$, $wR_2 = 0.0527$, 4258 reflections of which 2668 were independent with $R_{\text{int}} = 0.0361$.

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