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Diels–Alder Reactions of 5,6-Dihydrothiazolo[3,2-*d*][1,4,2]diazaphospholes: A DFT Investigation

Raj K. Bansal, Neelima Gupta, Surendra K. Kumawat, and Raakhi Gupta

Department of Chemistry, University of Rajasthan, Jaipur 302 004, India

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ABSTRACT: *The density functional theory level (B3LYP/6-311G**) computations of the Diels–Alder (DA) reactions of 5,6-dihydrothiazolo[3,2-d][1,4,2]-diazaphospholes with 1,3-butadiene and with isoprene confirm pericyclic mechanism via asynchronous transition states. The aromatic character of the transition states is established by negative nucleus independent chemical shift (NICS) values falling in the range from −14 to −16. Integration of the dienophilic >C=P− functionality in the 6π aromatic azaphosphole ring raises the activation energy barrier (B3LYP/6-311++G**//B3LYP/6-311G**) compared to that for the DA reaction of the acyclic phosphaethene, but it is lower than the activation energy barrier for the DA reaction of the corresponding 10π aromatic system, thiazolo[3,2-d][1,4,2]diazaphospholes. The experimentally observed stereo- and regioselectivities in the reactions can be accounted on the basis of secondary molecular orbital (SMO) interactions detected in the respective transition structures. The attachment of an electron-withdrawing group to the dienophilic moiety enhances both stereo- and regioselectivities which agree well with the experimental values. Solvent (toluene) effect studied with polarizable continuum model (PCM) indicates that the stereo- and regioselectivities are not affected by the solvent.* © 2006 Wiley Periodicals, Inc. Heteroatom Chem 17:402–410, 2006; Published online in Wiley InterScience (www.interscience.wiley.com). DOI 10.1002/hc.20196

Correspondence to: Raj K. Bansal; e-mail: rajbns@yahoo.com.
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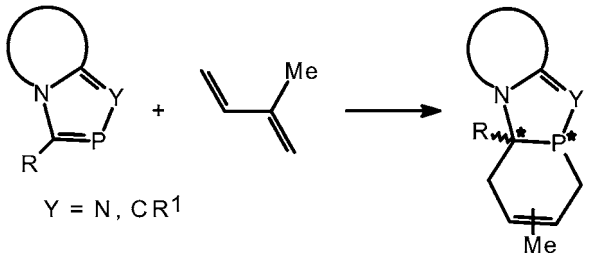
INTRODUCTION

The Diels–Alder (DA) reaction constitutes one of the important methods for the synthesis of the six-membered rings [1]. An analogy between the 6π electrons of benzene and six electrons in the cyclic transition state of the DA reaction of butadiene and ethylene was recognized [2]. The prototype DA reaction between butadiene and ethylene has been investigated theoretically at different levels [3]. Schleyer and coworkers [4] applied magnetic properties as criteria to establish aromatic nature of the transition states in the DA reactions of ethylene with butadiene and with cyclopentadiene. The horizon of the DA reaction has been further broadened by extending it to the organophosphorus compounds having >C=P− functionality, such as heterophospholes [5], anellated azaphospholes [6], phosphinines [7], and phosphaalkenes [8]. In fact, successful accomplishment of these reactions endorses the proposition, "phosphorus is a carbon copy of carbon" [9]. We have reported the synthesis of a variety of anellated azaphospholes through three methods, namely, [4 + 1] cyclocondensation [6], [3 + 2] cyclocondensation [10], and 1,5-electrocyclization [11]. The DA reaction of the >C=P− functionality in these molecules generates two stereogenic centers in one



SCHEME 1

step (Scheme 1). Stereo- and regioselectivities accompanying these reactions are the other important features [12]. We have undertaken a systematic investigation of the DA reactions of some of these compounds, both experimentally as well as theoretically. 1,3-Azaphospholo[5,1-*a*]isoquinoline undergoes DA reaction with 2,3-dimethylbutadiene [13] and with isoprene [14] in the presence of sulfur or methyl iodide with complete *endo* stereoselectivity. The extent of regioselectivity in the reaction with isoprene, however, depends on the nature of the oxidizing agent, in the presence of sulfur it is 100%, whereas in the presence of methyl iodide it decreases to 62% [14]. These reactions could be accomplished under microwave irradiation in much shorter time without affecting the stereo- and regioselectivities [15]. The DA reactions of thiazolo[3,2-*d*][1,4,2]diazaphospholes and their 5,6-dihydro- and benzo-derivatives and those of 1,3-azaphospholo[5,1-*b*]benzothiazole occur with complete *endo* stereoselectivity, and in the reaction with isoprene, 70–100% regioselectivity is observed [16]. [1,4,2]Diazaphospholo[4,5-*a*]pyridines follow a similar course in their DA reactions with 2,3-dimethylbutadiene and with isoprene, 80% regioselectivity being observed in the latter case [17].

The experimental results of several DA reactions have been rationalized on the basis of computational calculations [18]. The theoretical studies of the DA reactions of the phosphorus-containing reactants, though reported so far scarcely, lead to the conclusion that they involve lower activation energy barriers relative to the analogous hydrocarbon systems due to the weaker C=P π bond as compared to the C=C π bond, although the exothermicities in the two cases are comparable [19,20]. The DFT calculations of the prototype DA reactions of phosphaethene with 1,3-butadiene and with isoprene at B3LYP/6-311+G** level confirmed a pericyclic mechanism, but indicated low regioselectivity, and in order to account for the experimentally observed high regioselectivity, an alternative radical-cation mechanism was proposed [20]. It has been reported that an aromatic stabilization process of the masked diene accelerates the DA reaction through an "early" TS, while dearomatization of a DA reactant deactivates the cycloaddition via a "late" TS [21]. In view of these findings, the prototype model of the DA reaction of the acyclic phosphaethene with 1,3-diene [20] was considered inadequate to explain all the aspects of the DA reaction of the aromatic azaphospholes having the dienophilic moiety >C=P– integrated in the aromatic sextet, and we undertook a systematic theoretical study of these reactions at the DFT level to investigate the origin of the observed stereo- and regioselectivities. We have recently reported that dearomatization of the azaphosphole ring accompanying DA reaction of the 10π thiazolo[3,2-*d*][1,4,2]diazaphospholes raises the activation energy barrier by 4–5 kcal mol^{-1} as compared to those for the DA reactions of the acyclic phosphaethene, and the ratios of the *endo/exo* stereoisomers and *meta* (P/Me, 1:3)/*para* (P/Me, 1:4) regioisomers computed from the Boltzmann distribution are in very good agreement with the experimental values [22].

We have now computed the DA reactions of the 6π aromatic system, 5,6-dihydrothiazolo[3,2-*d*]-[1,4,2]diazaphospholes with 1,3-butadiene and with isoprene at DFT level (B3LYP/6-311++G**//B3LYP/6-311G**) to evaluate origin of the stereo- and regioselectivities reported experimentally [16] and also to compare the activation energy barriers with those for the 10π aromatic, thiazolo[3,2-*d*][1,4,2]-diazaphospholes and acyclic phosphaethene.

COMPUTATIONAL METHODS

Gaussian 03 package of programs [23] was used for the calculations. The geometries of the reactants, products, and the transition structures resulting from the DA reactions were optimized at the restricted Becke's three-parameter hybrid functional in conjunction with the correlation functional of Lee, Yang, and Parr (B3LYP) level with 6-311G** basis set. Vibrational frequencies were also calculated at the same level. All minima and transition structures were confirmed to have none or one imaginary frequency, respectively. Total energies were calculated by adding unscaled zero-point energy (ZPE) from B3LYP/6-311G** level to the single point energies calculated at B3LYP/6-311++G** level. The NICS values were calculated at GIAO-B3LYP/6-311++G**//B3LYP/6-311G** level [24]. The interrelation between the respective reactants, transition structures, and products was established by carrying out intrinsic reaction coordinate (IRC) calculations. Natural bond orbital (NBO) analysis [25] was done for determining the bond order (Wiberg bond indices) [26] of the transition structures.

The effect of the solvent (toluene) has been investigated by computing single point energy of the gas phase optimized geometries (B3LYP/6-311G**) at B3LYP/6-311++G** level with SCRF method [27] based on Tomasi's integrated equation formalism polarizable continuum model (IEFPCM) [28] and adding to it the unscaled ZPE calculated at B3LYP/6-311G** level for the gas phase.

RESULTS AND DISCUSSION

We have computed nine model DA reactions of 5,6-dihydrothiazolo[3,2-*d*][1,4,2] diazaphospholes **1**, including the one of the non-phosphorus analogue **2**, with 1,3-butadiene **3** and isoprene **4** that are summarized in Table 1.

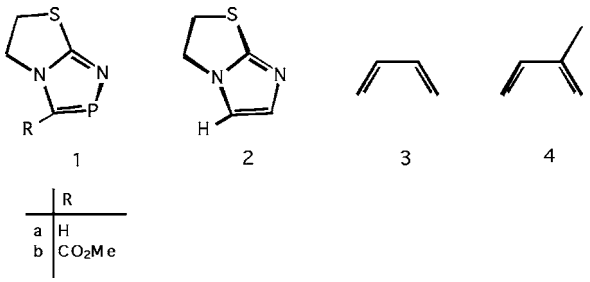
Geometries and NICS Values

The B3LYP/6-311G** optimized geometries of the transition structures (TS_1–TS_9) are given in Fig. 1 along with the bond distances (in Å) and Wiberg bond indices (in parenthesis) of the two new forming bonds. The respective nucleus independent chemical shift (NICS) value (in ppm) [29] is also shown for each transition structure. The negative NICS values (from −14 to −16) establish aromatic character of the transition structures [29] which indicates that all the DA reactions follow a pericyclic mechanism. The transition structures are, however, asynchronous, the forming P2—C9 bond being more advanced (WBI = 0.42–0.55) than the C3—C12 bond (WBI = 0.24–0.34). In the case of the DA reactions of 3-methoxycarbonyl-5,6-dihydrothiazolo[3,2-*d*]-[1,4,2]diazaphosphole, asynchronicity of the forming bonds increases further, possibly due to the steric hindrance caused by the ester group.

3-Methoxycarbonyl-5,6-dihydrothiazolo[3,2-*d*][1,4,2]diazaphosphole (**1b**) can exist in two conformational forms resulting from rotation around C3—C9 bond. In fact, two minima corresponding to these conformers **1bA** and **1bB** are located on the potential energy surface which are separated by an energy barrier of 8.96 kcal mol^{-1}. The optimized geometries (B3LYP/6-311G**) of **1bA** and **1bB** and of the transition structure are given in Fig. 2.

The conformer **1bA** (torsion angle PCCO = 177.9°) is more stable than **1bB** (torsion angle PCCO = −1.1°) by 2.77 kcal mol^{-1}. The greater stability of **1bA** having C=P and C=O moieties in the antiperiplanar orientation could be rationalized by NBO analysis which revealed increased $\pi_{P2-C3} \rightarrow \pi^*_{C9-O10'}$, $LP_{O11} \rightarrow \pi^*_{C9-O10}$ and $\pi^*_{P2-C3} \rightarrow \pi^*_{C9-O10}$ interactions.

TABLE 1 Investigated DA Reactions of **1** and **2**



Reaction No.	Reactants (Approach)	TS	Product
1	**1a** + **3** (*Endo*)	TS_1	P_1
2	**1a** + **3** (*Exo*)	TS_2	P_2
3	**1a** + **4** (*Endo*)	TS_3	P_3 (P/Me, 1:3)
4	**1a** + **4** (*Endo*)	TS_4	P_4 (P/Me, 1:4)
5	**1b** + **3** (*Endo*)	TS_5	P_5
6	**1b** + **3** (*Exo*)	TS_6	P_6
7	**1b** + **4** (*Endo*)	TS_7	P_7 (P/Me, 1:3)
8	**1b** + **4** (*Endo*)	TS_8	P_8 (P/Me, 1:4)
9	**2** + **3** (*Endo*)	TS_9	P_9

Energetics

The total energies (B3LYP/6-311++G**//B3LYP/6-311G**), activation (ΔE_a), and reaction (ΔE_{rxn}) energies of the reactions 1–9 are given in Table 2.

It may be noted that although the exothermicities of the DA reactions of 5,6-dihydrothiazolo[3,2-*d*][1,4,2]diazaphospholes **1** and that of its non-phosphorus analogue **2** are comparable, the activation energy barrier for the former is lower than that for the latter by 13.08 kcal mol^{-1}. It is in conformity with the earlier results which led to the conclusion that introduction of phosphorus in a DA reactant lowers the activation barrier due to weaker C=P π bond relative to the C=C π bond [19,20].

It has been reported that dearomatization accompanying a DA reaction raises its activation energy barrier [21]. In view of this, the activation energies for the DA reactions of three dienophiles, namely thiazolo[3,2-*d*][1,4,2]diazaphosphole **5** (10π aromatic), 5,6-dihydrothiazolo[3,2-*d*][1,4,2]diazaphosphole **1** (6π aromatic), and acyclic phosphaethene **6** with a 1,3-diene are expected to decrease in the order **5** > **1** > **6**. In fact the ΔE_a, for the DA reaction of 5,6-dihydrothiazolo[3,2-*d*][1,4,2]diazaphosphole **1a** with 1,3-butadiene, is found to be higher than for the DA reaction of phosphaehene (calculated at B3LYP/6-311+G**//B3LYP/6-31G*) [20] by 5.62 kcal mol^{-1}, but lower than for the DA reaction of thiazolo[3,2-*d*][1,4,2]diazaphosphole (calculated at B3LYP/6-311++G**//B3LYP/6-311G**) [22] by 0.29 kcal mol^{-1}.

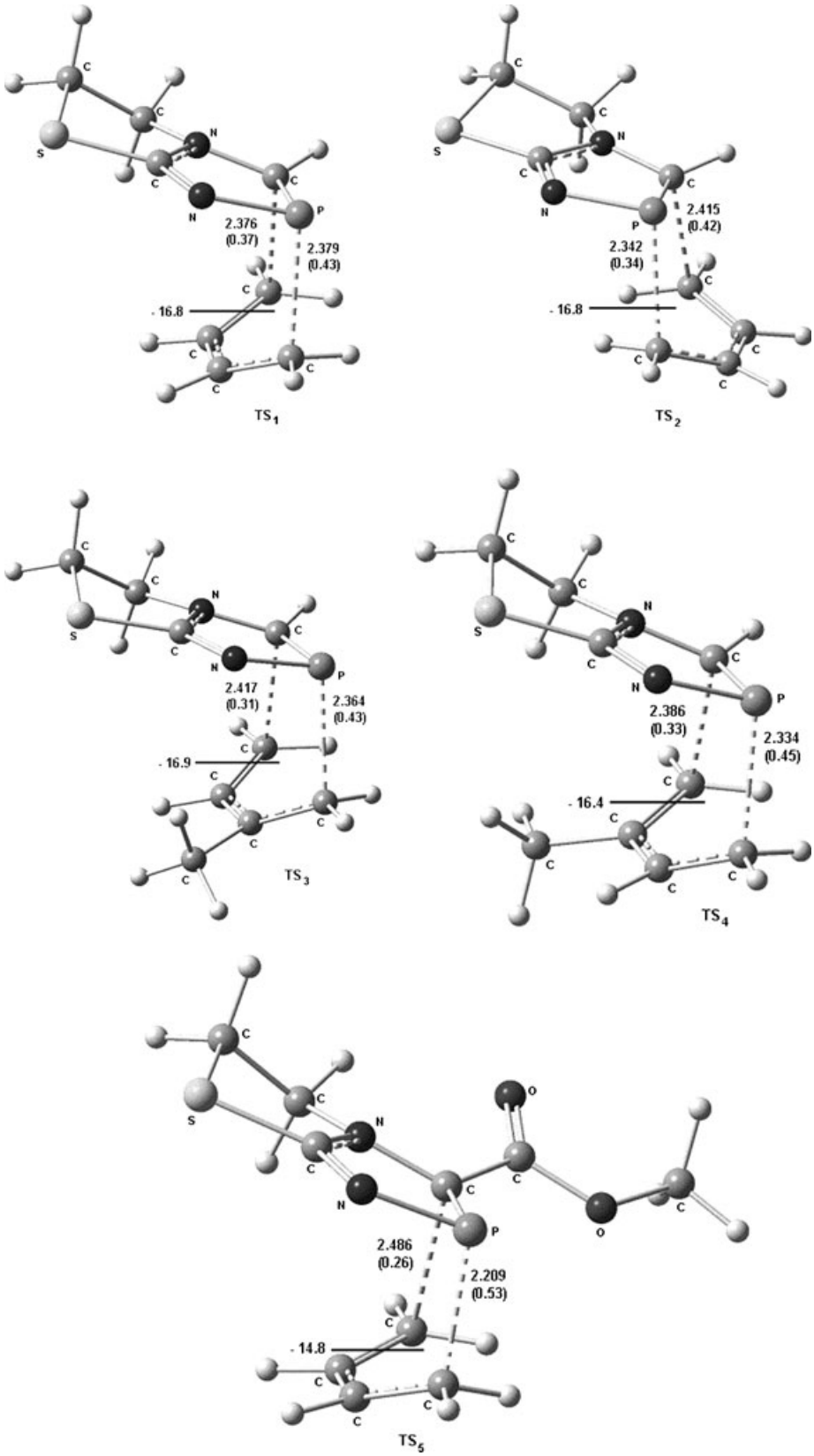


FIGURE 1 Optimized geometries (B3LYP/6-311G**) of the transition structures (TS_1—TS_5), bond distances (in Å), Wiberg bond indices (in parenthesis), and NICS values (in ppm).

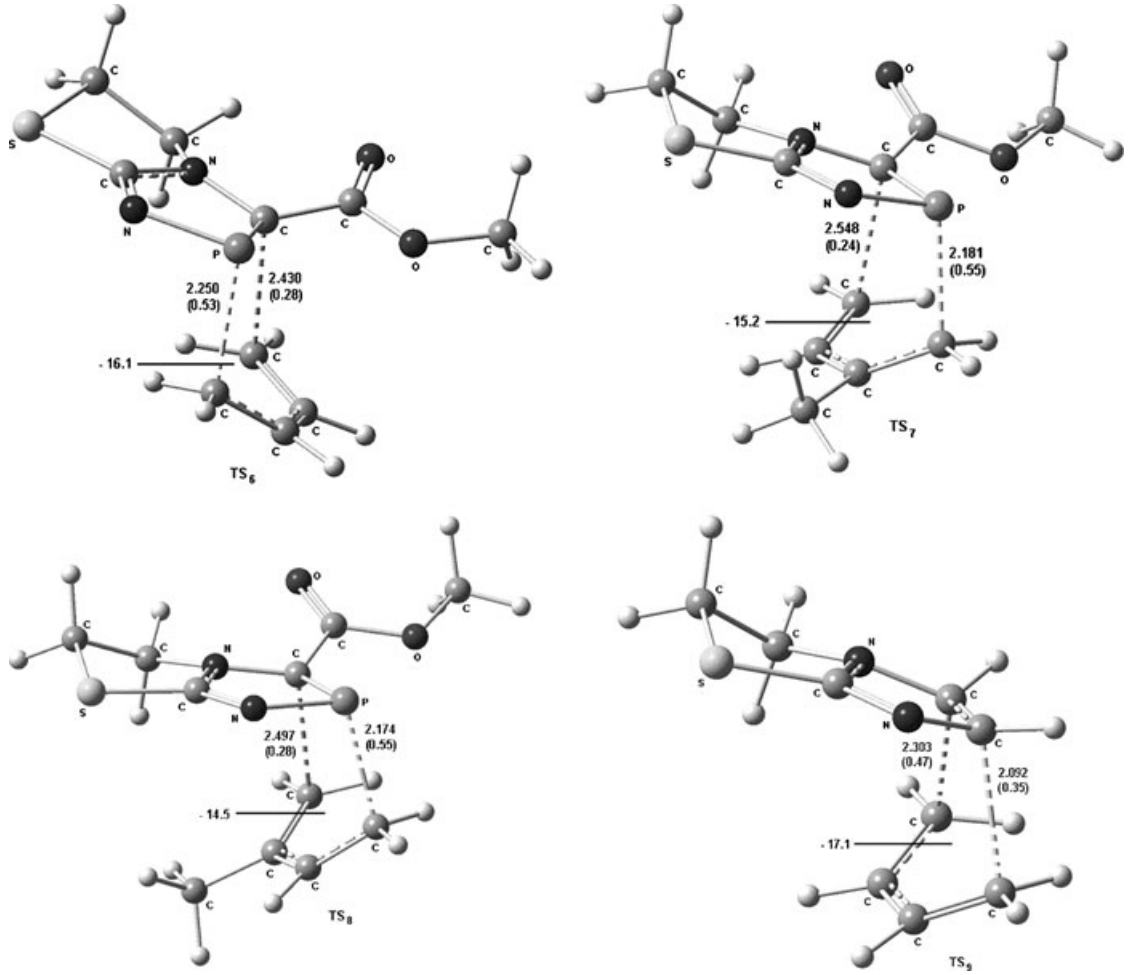


FIGURE 1 Continued

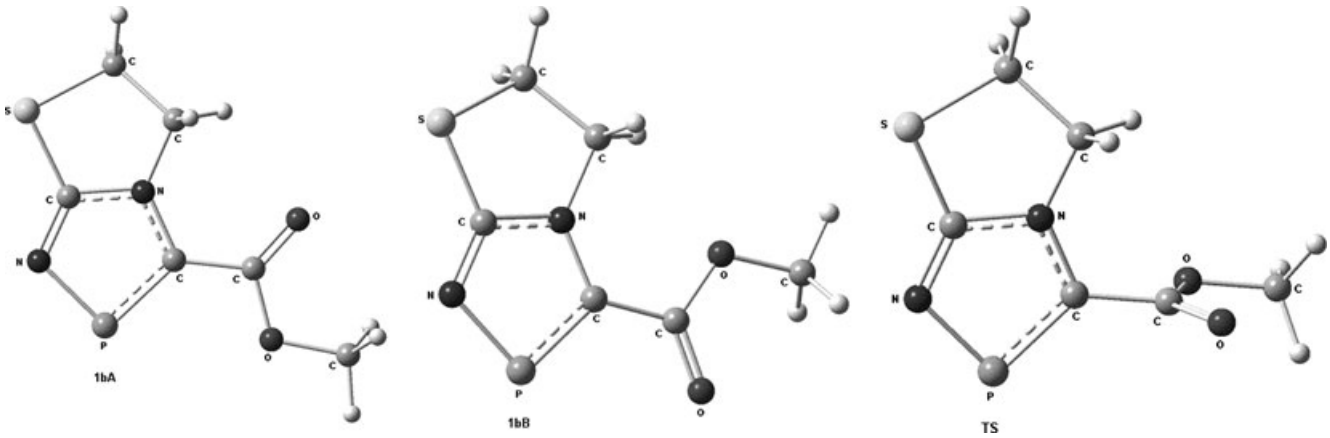


FIGURE 2 Optimized geometries (B3LYP/6-311G**) of the two conformers of **1b** and the corresponding TS.

TABLE 2 Total Energies and Relative Energies for the Stationary Points Corresponding to DA Reactions 1—9

	Total Energies[a] *(a.u.)*		*Relative Energies (kcal mol*$^{-1}$*)*	
	Gas Phase	*Toluene*	*Gas Phase*	*Toluene*
1a	−1004.502468	−1004.508760	0.0	0.0
1bA	−1232.409637	−1232.415455	0.0	0.0
1bB	−1232.405293	−1232.412064	2.72	2.13
TS[b]	−1232.395365	−1232.402588	8.96	8.07
2	−701.818335	−701.824806	0.0	0.0
3	−155.950050	−155.951692	0.0	0.0
4	−195.250518	−195.251835	0.0	0.0
TS_1	−1160.423778	−1160.430353	18.03	18.89
P_1	−1160.476829	−1160.483207	−15.26	−14.28
TS_2	−1160.422692	−1160.429138	18.72	19.65
P_2	−1160.474927	−1160.481233	−14.06	−13.04
TS_3	−1199.725428	−1199.731300	17.29	18.38
P_3	−1199.779428	−1199.785187	−16.59	−15.43
TS_4	−1199.723635	−1199.729742	18.42	19.36
P_4	−1199.777641	−1199.783714	−15.47	−14.51
TS_5	−1388.334581	−1388.341266	15.75	16.24
P_5	−1388.376555	−1388.383723	−10.58	−10.40
TS_6	−1388.331233	−1388.338007	17.86	18.28
P_6	−1388.372932	−1388.380142	−8.31	−8.15
TS_7	−1427.637054	−1427.643116	14.50	15.17
P_7	−1427.679259	−1427.685871	−11.99	−11.66
TS_8	−1427.633679	−1427.639969	16.61	17.14
P_8	−1427.677511	−1427.684265	−10.89	−10.65
TS_9	−857.718804	−857.725385	31.11	32.07
P_9	−857.789054	−857.795031	−12.97	−11.63

[a]Energies at B3LYP/6-311++G** + ZPE at B3LYP/6-311G** level.
[b]TS (**1bA** → **1bB**).

Stereo- and Regioselectivities

The observed *endo/exo* stereoselectivity can be explained on the basis of secondary molecular orbital (SMO) interactions detectable in the highest occupied molecular orbitals (HOMO) of the transition structures, TS_1 and TS_5 (Fig. 3).

Appreciable SMO interactions can be expected between C10—C11 (π) and N1—C8—N4 (π) orbitals due to their proximity and similar phases. These interactions are, however, missing in the transition structures TS_2 and TS_6 resulting from the *exo* approach.

Similarly, the exclusive formation of the *meta* regioisomer (P/Me, 1:3) in the DA reaction of 3-methoxycarbonyl-5,6-dihydrothiazolo[3,2-d][1,4,2]-diazaphosphole (**1b**) with isoprene [16] can be rationalized on the basis of the SMO interactions observed in the HOMO of the transition structure TS_7 (Fig. 4). It can be seen that the orbital having lone pair on sulfur and the *p*-orbital on the methyl carbon with similar phase are quite close. On the other hand, this SMO interaction is missing in the transition structure TS_8 resulting from the *para* approach of **1b** and isoprene.

The ratios of the regio- and stereoisomers in the DA reactions of vinylboranes have been calculated from the Boltzmann distribution [30], and the values so obtained were found in good agreement with the experimental results. Experimentally, we have observed earlier that 3-alkoxycarbonyl-5,6-dihydrothiazolo[3,2-*d*][1,4,2]diazaphosphole exhibits complete *endo* stereoselectivity in its DA reactions [16]. Furthermore, *meta* regioproduct (P/Me, 1:3) was formed exclusively in its reaction with isoprene. The calculated ratios of the *endo*/*exo* stereoisomers and of the *meta* (P/Me, 1:3)/*para* (P/Me, 1:4) regioisomers are given in Table 3. It can be seen that the computed ratios for the *endo*/*exo* stereoisomers and also for the *meta* (P/Me, 1:3) /*para* (P/Me, 1:4) regioisomers agree nicely with the experimental values reported for the 3-alkoxy substituted 5,6-dihydrothiazolo[3,2-*d*][1,4,2]diazaphosphole. The experimental stereoselectivity and regioselectivity results for the DA reactions of the 3-unsubstituted 5,6-dihydrothiazolo[3,2-*d*][1,4,2]diazaphosphole have not been reported so far. The theoretical calculations predict approximately 76% *endo* stereoselectivity and a similar extent of preference for the *meta* regioproduct.

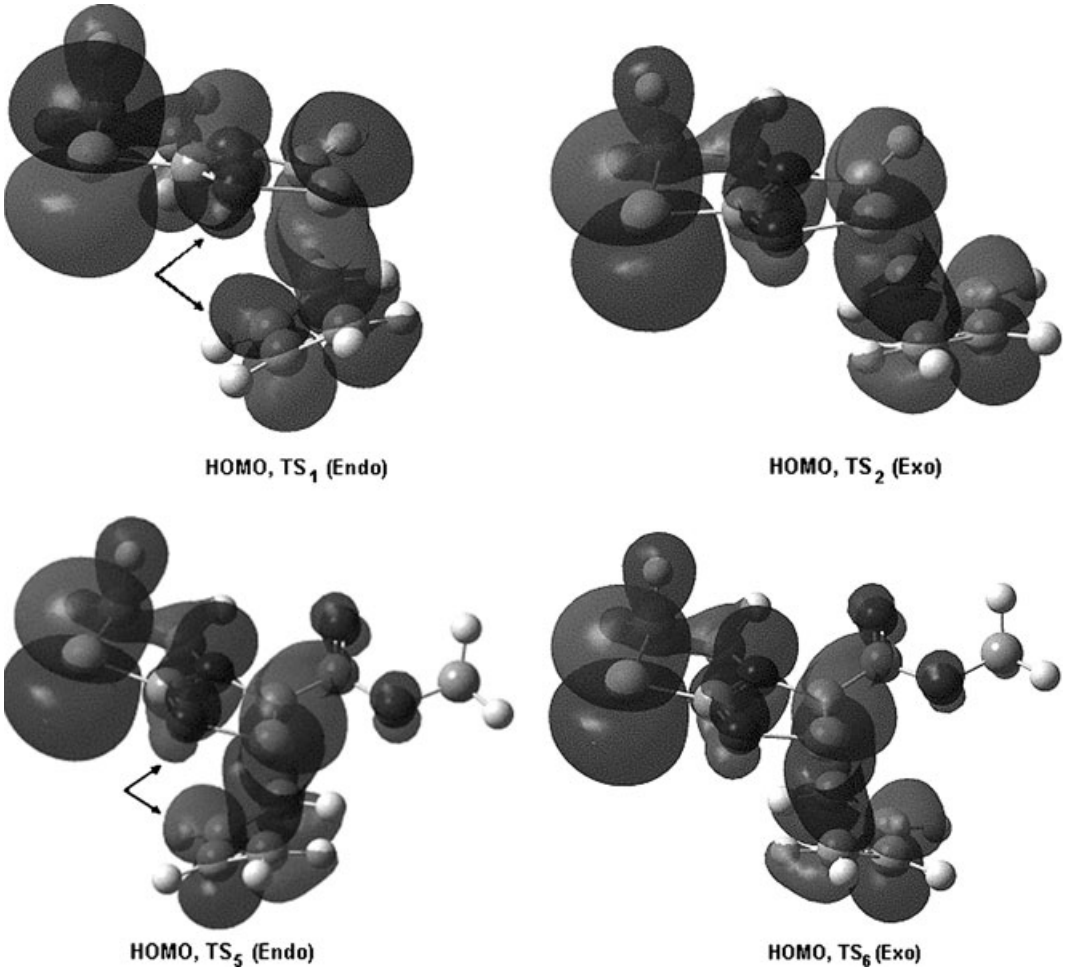


FIGURE 3 Secondary molecular orbital interactions in *endo* transition structures for DA reactions of 5,6-dihydrothiazolo[3,2-*d*][1,4,2]diazaphospholes (**1**).

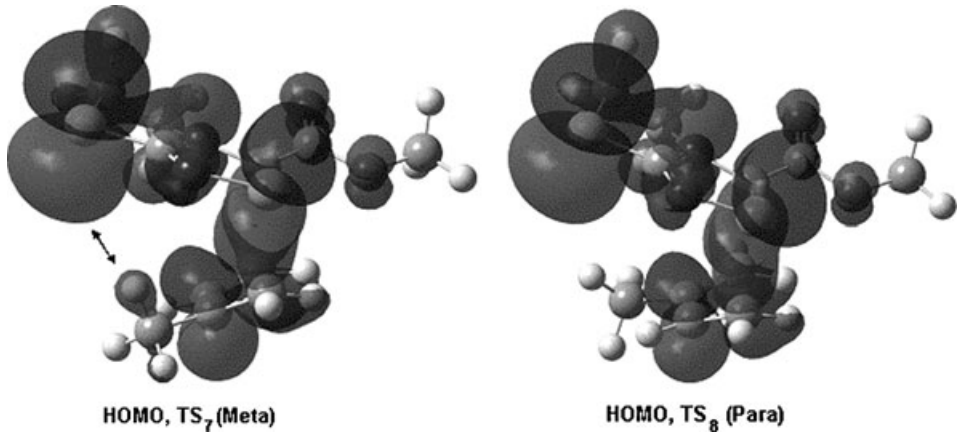


FIGURE 4 Secondary molecular orbital interaction in the **meta** transition structure for DA reaction of 5,6-dihydrothiazolo[3,2-*d*][1,4,2]diazaphosphole **1b** with isoprene.

TABLE 3 Experimental and Calculated[a] Ratios of Stereoselectivity and Regioselectivity for the DA Reactions between Diazaphospholes **1** and Dienes **3, 4**

	Stereoselectivity (Endo : Exo)			*Regioselectivity (Meta : Para)*		
	Calculated			*Calculated*		
	Gas Phase	*Toluene*	*Experimental*	*Gas Phase*	*Toluene*	*Experimental*
1a	76:24	78:22	—	87:13	84:16	—
1b	97:03	97:03	100:0	97:03	97:03	100:0

[a]Products ratios were computed from the Boltzmann equation: $k_1/k_2 = e^{-\Delta E/RT}$, where ΔE is the difference between the calculated activation energies for the two processes, $T = 298.15$ K and $R = 1.9872$ cal K^{-1} mol^{-1}.

Computations of the solvent effect (toluene) reveal that toluene does not influence stereo- and regioselectivities.

It may be pointed out that NICS values of TS_3 and TS_7 corresponding to the preferred *meta* approach are more negative than for the TS_4 and TS_8 resulting from the *para* approach, indicating greater aromatic character of the former (Fig. 1). The differences are, however, small and inadequate to account for the 100% regioselectivity. Moreover, it has also been pointed out that although aromaticity of the transition state in the DA reaction is important, it does not determine regioselectivity [31].

CONCLUSION

The DA reactions of 5,6-dihydrothiazolo[3,2-*d*]-[1,4,2]diazaphosphole with 1,3-dienes follow a concerted mechanism, involving asynchronous transition states. Aromatic character of the transition structure is confirmed by negative NICS values. The activation energy barrier ($\Delta E_a = 14$–18 kcal mol^{-1}) is much lower than that for the DA reaction of the non-phosphorus analogue, 5,6-dihydroimidazo[2,1-*b*]thiazole confirming the fact that introduction of phosphorus in a DA reactant decreases the activation energy. The experimentally observed *endo* stereoselectivity as well as meta (P/Me, 1:3) regioselectivity can be rationalized on the basis of the SMO interactions detectable in the respective transition structures.

The calculated ratios of the *endo*/*exo* stereoisomers and also of the *meta*/*para* regioisomers are in good agreement with the experimental values. The computations with the solvent effect reveal that toluene does not influence *endo*/*exo* stereoselectivity or *meta*/*para* regioselectivity relative to those observed in the gaseous phase.

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