

## THEORETICAL STUDY OF THE TAUTOMERISM OF SUBSTITUTED AZAPHOSPHOLES

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**Abstract.** The heats of formation,  $\Delta H_f^\circ$ ; heats of tautomerization,  $\delta\Delta H_t^\circ$ ; dipole moments, and vertical ionization potentials of sixteen 2-, 4-, and 5-substituted 1,3-azaphospholes and the parent compound itself were calculated for isolated molecules and for molecules embedded into a dielectric medium, using semiempirical AM1 parametrization. Methyl-, carboxy-, formoxy-, and nitrogroups were used as substituents to azaphosphole ring carbon atoms. The solvent effect of dielectric medium was modelled by the self-consistent reaction field technique. The NH-form is predicted to be the predominant tautomer for all compounds in both media studied. However, in low dielectric media other tautomers may be present in some amount which can lead to alterations of reaction mechanisms in these media.

**Key words:** quantum chemistry, phosphorus, tautomerism.

### 1. INTRODUCTION

Various derivatives of 1,3-azaphosphole have been recently synthesized and studied spectroscopically [1–4]. As a new series of “phosphaaromatic” compounds they are of considerable interest both from the theoretical point of view and for practical applications. The geometry, electronic structure, and photoelectron spectrum of 1,3-azaphosphole and homologous azaarsole have been studied by *ab initio* SCF method using a medium-sized basis set (4-31G for P) [5].

In the present work we present the results of a systematic study of the electronic structure and energetics of NH-, PH-, 2H-, 4H-, and 5H-tautomers of 2-, 4-, and 5-substituted 1,3-azaphospholes using quantum-chemical LCAO MO SCF method with semiempirical AM1 parametrization [6,7]. The calculations were carried out for two media. One of them corresponds to isolated molecules (i.e. gas phase at low temperature and pressure), the other to a polarizable dielectric medium with the dielectric constant corresponding to that of water at room temperature ( $\epsilon=80$ ). The effect of the latter medium on the electronic structure of the solute was modelled by using the self-consistent reaction field (SCRF) Hamiltonian in MO calculations. Full relaxation of solvent in the field of solute (azaphosphole) molecule was assumed (cf. [8,9]). Methyl-, carboxy-, formoxy-, and nitrogroups were used as substituents to the ring of parent 1,3-azaphosphole.



## 2. RESULTS AND DISCUSSION

To our knowledge, there are no experimental data on the geometrical structure of 1,3-azaphosphole and its derivatives yet. However, we can compare the results of our calculations with the results of *ab initio* SCF LCAO MO calculations with the split-valence 4-31G basis set augmented by one set of polarization functions on phosphorus [5]. The comparison of geometrical data for 1,3-azaphosphole is presented in Table 1. The calculated bond lengths are reasonable by using both AM1 and PM3 [10] parametrizations (the 4-31G calculated bond lengths for phosphole and its analogs tend to be longer by 0.03–0.04 Å, cf. [5]). The bond angles are very similar to those of *ab initio* calculations. It is important to notice that the NH-tautomer is planar whereas in the PH-tautomer the phosphorus atom is turned out of the plane defined by other ring atoms by about 5 degrees. A similar structural feature was observed also for phosphole and thus both these ring systems can be considered as non-aromatic [11].

The AM1 calculated heats of formation  $\Delta H_f^0$ , dipole moments, and ionization potentials of 2-, 4-, and 5-substituted azaphospholes are given in Tables 2–7. The calculated tautomerization energies of the compounds are given in Tables 8–10.

As a rule, the calculated dipole moments are enhanced in the medium of dielectric constant  $\epsilon=80$ . This is also reflected in the electrostatic stabilization of the polar structures of molecules and an increase of solvation energy. The electrostatic stabilization energy has no simple (proportional) relation to the dipole moment value of solute molecule. However, a parallelism in dipole moment and solvation energy values can be observed.

In most cases, the tautomer of the largest dipole moment is the NH-tautomer. Correspondingly it has been characterized by the highest value of solvation (stabilization) energy and the relative stability of this form increases in comparison with other tautomers in a medium with a high dielectric constant. Because of small entropy effects the tautomeric equilibrium can be expected to shift towards the NH-tautomer in this medium. However, the order of stability of other tautomers may depend on the substituent at the azaphosphole ring and on the surrounding medium.

In 2-substituted azaphospholes the second next stable tautomer is the 4H-form of molecules whereas in the unsubstituted compound the second next stable tautomer is its 2H-form. These orders of stability are valid both in gas phase ( $\epsilon=1$ ) and in the medium with a high dielectric constant ( $\epsilon=80$ ). In 4-substituted azaphospholes the 4H-form is the second next stable tautomer only in the case of some electron-accepting substituents (carboxy- and nitrogroups). In 4-methylazaphosphole and 4-formoxyazaphosphole the second next stable tautomer is their 2H-form. In 5-substituted azaphospholes the second next stable tautomer is again the 4H-form, in both media studied. In most cases of 2-, 4-, and 5-substituted tautomers and in the case of unsubstituted compound the least stable form is the PH-tautomer.

In general, the order of stability of various tautomers remains unchanged in different media. However, the relative stability of 4H- and 5H-forms of 4-nitroazaphosphole is reversed in the medium with a high dielectric constant in comparison with that for isolated molecules. The same can be observed in the case of PH- and 5H-forms of 5-formoxy- and 5-nitroazaphospholes.

Table 1

*Ab initio* [<sup>5</sup>], PM3<sup>a</sup>, and AM1<sup>a</sup> SCF (SCRF) LCAO MO calculated geometries of the NH- and PH-tautomers of 1,3-azaphosphole

Geometrical variable <sup>b</sup>	NH-tautomer			PH-tautomer		
	4-31G	PM3	AM1	4-31G	PM3	AM1
1(P—C2)	1.698	1.714	1.621	1.837	1.851	1.736
1(C2—N)	1.361	1.373	1.368	1.275	1.298	1.300
1(N—C4)	1.365	1.377	1.370	1.424	1.372	1.377
1(C4—C5)	1.353	1.371	1.378	1.329	1.343	1.357
1(P—C5)	1.772	1.751	1.660	1.814	1.823	1.706
∠(C2PC5)	88.9	91.2	94.8	86.4	87.8	91.5
∠(NC2P)	113.1	111.4	111.7	114.3	111.8	113.3
∠(C2NC4)	114.8	112.2	112.1	112.1	112.3	112.0
∠(NC4C5)	112.1	110.7	111.1	116.6	111.9	112.9
∠(C4C5P)	111.7	110.9	109.7	110.2	109.6	108.5

<sup>a</sup> Present work.

<sup>b</sup> Bond lengths are given in ångströms and bond angles in degrees.

Table 2

AM1 SCF calculated heats of formation,  $-\Delta H_f^0$ , dipole moments,  $\mu$ , and ionization potentials, IP, for the isolated molecules of different tautomers of 2-substituted azaphospholes

Substituent	Tautomer	$-\Delta H_f^0$ , kcal/mol	$\mu$ , D	IP, eV
—H	NH	36.036	4.076	8.916
	PH	56.733	1.763	9.819
	2H	46.141	2.036	9.650
	4H	49.291	0.875	10.093
	5H	52.746	1.714	10.170
2—CH <sub>3</sub>	NH	33.391	3.994	8.667
	PH	52.917	1.684	9.642
	2H	49.410	0.793	10.021
	4H	41.318	1.586	9.386
	5H	50.399	1.247	10.053
2—COOH	NH	—46.937	4.676	9.462
	PH	—23.389	3.375	10.166
	2H	—29.649	3.066	10.509
	4H	—34.861	3.851	10.086
	5H	—34.855	3.840	10.087
2—CHO	NH	5.840	2.912	9.392
	PH	33.254	2.693	10.041
	2H	26.982	3.617	10.450
	4H	20.930	4.425	10.124
	5H	29.658	3.798	10.352
2—NO <sub>2</sub>	NH	51.634	6.001	9.961
	PH	77.121	5.186	10.437
	2H	67.284	5.636	11.001
	4H	65.636	6.677	10.545
	5H	70.328	6.193	10.987



Table 3

AMI SCF calculated heats of formation,  $\Delta H_f^0$ , dipole moments,  $\mu$ , and ionization potentials, IP, of different tautomers of 2-substituted azaphospholes in dielectric medium with  $\epsilon=80$  (aqueous solution)

Substituent	Tautomer	$\Delta H_f^0$ , kcal/mol	$\mu$ , D	IP, eV
—H	NH	27.690	5.495	8.540
	PH	57.828	3.392	8.392
	2H	44.272	2.539	9.581
	4H	48.929	1.124	10.067
	5H	51.302	2.260	10.077
2—CH <sub>3</sub>	NH	28.160	4.940	8.437
	PH	52.092	1.928	9.704
	2H	49.207	0.970	10.012
	4H	40.520	1.920	9.339
	5H	49.876	1.568	10.046
2—COOH	NH	-53.336	5.715	9.263
	PH	-26.474	3.924	10.237
	2H	-32.503	3.836	10.490
	4H	-39.216	4.717	10.102
	5H	-39.469	4.992	10.106
2—CHO	NH	3.082	3.582	9.318
	PH	30.956	3.258	10.110
	2H	22.512	4.593	10.470
	4H	14.028	5.732	10.156
	5H	24.933	6.696	10.406
2—NO <sub>2</sub>	NH	40.954	7.399	9.844
	PH	57.678	7.867	10.907
	2H	58.048	6.861	11.021
	4H	57.987	8.211	10.872
	5H	58.667	7.756	10.901

Table 4

AMI SCF calculated heats of formation,  $\Delta H_f^0$ , dipole moments,  $\mu$ , and ionization potentials, IP, for the isolated molecules of different tautomers of 4-substituted azaphospholes

Substituent	Tautomer	$\Delta H_f^0$ , kcal/mol	$\mu$ , D	IP, eV
1	2	3	4	5
4—CH <sub>3</sub>	NH	33.575	3.865	8.880
	PH	52.441	1.995	9.629
	2H	44.082	1.355	9.754
	4H	45.760	1.996	9.622
	5H	47.357	2.156	9.763

Table 4 (continued)

1	2	3	4	5
4-COOH	NH	-47.933	5.389	9.368
	PH	-26.599	1.194	10.192
	2H	-33.473	1.514	10.547
	4H	-33.811	1.683	10.063
	5H	-30.181	1.452	10.547
4-CHO	NH	6.474	4.943	9.366
	PH	29.638	3.082	10.171
	2H	22.014	2.447	10.466
	4H	30.537	3.203	9.734
	5H	25.611	1.579	10.538
4-NO <sub>2</sub>	NH	49.659	7.766	9.797
	PH	71.689	4.078	10.462
	2H	63.442	4.126	11.048
	4H	66.483	3.463	10.372
	5H	66.682	3.592	11.026

Table 5

AMI SCRFF calculated heats of formation,  $\Delta H_f^0$ , dipole moments,  $\mu$ , and ionization potentials, IP, for different tautomers of 4-substituted azaphospholes in dielectric medium with  $\epsilon=80$  (aqueous solution)

Substituent	Tautomer	$\Delta H_f^0$ , kcal/mol	$\mu$ , D	IP, eV
4-CH <sub>3</sub>	NH	28.652	4.795	8.670
	PH	51.254	2.321	9.667
	2H	43.460	1.711	9.703
	4H	44.512	2.397	9.567
	5H	45.764	2.743	9.650
4-COOH	NH	-56.537	6.638	9.174
	PH	-27.004	1.432	10.221
	2H	-34.107	1.784	10.559
	4H	-34.631	2.042	9.997
	5H	-30.733	1.652	10.521
4-CHO	NH	-1.830	6.256	9.242
	PH	26.579	3.768	10.302
	2H	19.824	3.244	10.610
	4H	27.332	3.841	9.621
	5H	24.676	2.127	10.597
4-NO <sub>2</sub>	NH	31.444	9.686	9.659
	PH	66.904	4.930	10.512
	2H	58.395	5.084	11.122
	4H	63.376	3.911	10.352
	5H	63.025	4.301	11.021



Table 6

AM1 SCRF calculated heats of formation,  $\Delta H_f^0$ , dipole moments,  $\mu$ , and ionization potentials, IP, for the isolated molecules of different tautomers of 5-substituted azaphospholes

Substituent	Tautomer	$\Delta H_f^0$ , kcal/mol	$\mu$ , D	IP, eV
5-CH <sub>3</sub>	NH	28.352	4.200	8.745
	PH	48.741	1.580	9.569
	2H	41.859	1.291	10.013
	4H	38.182	2.527	9.409
	5H	48.828	1.772	10.107
5-COOH	NH	-54.595	4.009	9.404
	PH	-29.451	2.550	10.266
	2H	-35.066	1.291	10.447
	4H	-38.187	0.997	10.048
	5H	-31.175	0.999	10.508
5-CHO	NH	2.436	1.033	9.294
	PH	26.933	2.792	10.121
	2H	21.835	1.746	10.307
	4H	18.590	0.676	9.903
	5H	26.685	0.930	10.385
5-NO <sub>2</sub>	NH	41.415	3.759	9.873
	PH	66.256	5.761	10.701
	2H	61.564	4.005	10.920
	4H	58.462	3.487	10.504
	5H	63.631	3.921	10.925

Table 7

AM1 SCRF calculated heats of formation,  $\Delta H_f^0$ , dipole moments,  $\mu$ , and ionization potentials, IP, of different tautomers of 5-substituted azaphospholes in dielectric medium with  $\epsilon=80$  (aqueous solution)

Substituent	Tautomer	$\Delta H_f^0$ , kcal/mol	$\mu$ , D	IP, eV
1	2	3	4	5
5-CH <sub>3</sub>	NH	22.462	5.255	8.443
	PH	48.027	1.787	9.602
	2H	41.301	1.618	9.968
	4H	47.517	2.703	9.626
	5H	47.778	2.220	10.056
5-COOH	NH	-59.271	4.881	9.253
	PH	-31.410	3.176	10.397
	2H	-35.537	1.543	10.484
	4H	-38.431	1.085	10.063
	5H	-31.476	1.243	10.548

1	2	3	4	5
5-CHO	NH	2.072	1.311	9.231
	PH	24.381	3.451	10.268
	2H	20.831	2.167	10.319
	4H	18.442	0.828	9.903
	5H	26.385	1.190	10.426
5-NO <sub>2</sub>	NH	37.249	4.616	9.947
	PH	55.981	7.302	10.990
	2H	56.480	5.151	11.149
	4H	54.476	4.583	10.737
	5H	59.231	4.727	11.042

Table 8

AM1 SCF and AM1 SCRF calculated tautomerization heats,  $\delta\Delta H_t^0$ , of different tautomers of 2-substituted azaphospholes in two different dielectric media

Substituent	Tautomer	$\delta\Delta H_t^0$ ( $\epsilon=1$ ), kcal/mol	$\delta\Delta H_t^0$ ( $\epsilon=80$ ), kcal/mol
—H	NH	(0)	(0)
	PH	20.697	—
	2H	10.105	16.582
	4H	13.255	21.329
	5H	16.710	23.612
2-CH <sub>3</sub>	NH	(0)	(0)
	PH	19.526	23.932
	2H	16.019	21.047
	4H	7.927	12.360
	5H	17.008	21.716
2-COOH	NH	(0)	(0)
	PH	23.548	26.862
	2H	17.291	20.833
	4H	12.076	14.120
	5H	12.082	13.867
2-CHO	NH	(0)	(0)
	PH	27.417	27.874
	2H	21.142	19.430
	4H	15.090	10.946
	5H	23.818	21.851
2-NO <sub>2</sub>	NH	(0)	(0)
	PH	25.487	25.756
	2H	15.650	17.094
	4H	14.002	17.033
	5H	18.694	17.713

Table 9

AM1 SCF and AM1 SCRF calculated tautomerization heats,  $\delta\Delta H_t^0$ , of different tautomers of 4-substituted azaphospholes in two different dielectric media

Substituent	Tautomer	$\delta\Delta H_t^0$ ( $\epsilon=1$ ), kcal/mol	$\delta\Delta H_t^0$ ( $\epsilon=80$ ), kcal/mol
4-CH <sub>3</sub>	NH	(0)	(0)
	PH	18.866	22.602
	2H	10.507	14.808
	4H	12.185	15.860
	5H	13.782	17.112
4-COOH	NH	(0)	(0) <sup>c</sup>
	PH	21.334	29.533
	2H	14.460	22.430
	4H	14.122	21.906
	5H	17.752	25.804
4-CHO	NH	(0)	(0)
	PH	23.164	28.409
	2H	15.540	21.654
	4H	24.063	29.162
	5H	19.137	26.506
4-NO <sub>2</sub>	NH	(0)	(0)
	PH	22.030	35.460
	2H	13.783	26.951
	4H	16.824	34.932
	5H	17.023	31.581

Table 10

AM1 SCF and AM1 SCRF calculated tautomerization heats,  $\delta\Delta H_t^0$ , of different tautomers of 5-substituted azaphospholes in two different dielectric media

Substituent	Tautomer	$\delta\Delta H_t^0$ ( $\epsilon=1$ ), kcal/mol	$\delta\Delta H_t^0$ ( $\epsilon=80$ ), kcal/mol
5-CH <sub>3</sub>	NH	(0)	(0)
	PH	20.389	25.565
	2H	13.507	18.839
	4H	9.830	25.055
	5H	20.476	25.316
5-COOH	NH	(0)	(0)
	PH	25.144	27.861
	2H	19.529	23.734
	4H	16.408	20.840
	5H	23.420	27.795
5-CHO	NH	(0)	(0)
	PH	24.497	22.309
	2H	19.399	18.759
	4H	16.154	16.370
	5H	24.249	24.313
5-NO <sub>2</sub>	NH	(0)	(0)
	PH	24.841	18.732
	2H	20.149	19.231
	4H	17.047	17.227
	5H	22.216	21.982



### 3. CONCLUSIONS

Our results indicate that the presence of various tautomers of substituted azaphospholes cannot be neglected in discussions of the reactivity and reaction mechanism of these compounds, particularly in low dielectric media and in gas phase. Secondly, the PH-tautomer is usually of much higher energy than the predominant NH-tautomer and cannot be considered as competitive to it. Nevertheless, some CH-tautomers can compete with NH-tautomer, particularly in ring-substitution reactions due to substantial reordering of ring electron density in different tautomeric forms.

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### ASENDATUD ASAFOSFOOLIDE TAUTOMEERIA TEOREETILINE UURIMINE

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Kuueteistkümne 2-, 4- ja 5-asendatud asafosfooli tekkeentalpiad  $\Delta H_f^0$ , tautomerisatsioonientalpiad  $\delta\Delta H_f^0$ , dipoolmomendid ning vertikaalsed ionisatsioonipotentsiaalid arvutati kvantkeemilise AM1-meetodi abil gaasifaasis ning kõrge dielektrilise läbitavusega keskkonnas. Asendusrühmadena vaadeldi metüül-, formoksü- ning nitrorühma. Lahusti

mõju modelleeriti kooskõlalise reaktsioonivälja meetodi abil. Kõigi uuri-  
tud ühendite korral leiti, et tautomeerseks põhikomponendiks nii gaasi-  
faasis kui ka dielektriliselt polariseeritavas keskkonnas on molekuli  
NH-vorm. Madala dielektrilise läbitavusega keskkonnades võib märga-  
tavas koguses leiduda ka PH-vormi, mis mõjutab nende ühendite sum-  
maarset reaktsioonivõimet.

## ТЕОРЕТИЧЕСКОЕ ИССЛЕДОВАНИЕ ТАВТОМЕРИИ ЗАМЕЩЕННЫХ АЗАФOSFОЛОВ

Марек СТРАНДБЕРГ, Гюнтер П. ШИМЕНЦ, Мати КАРЕЛСОН

С помощью квантовохимического метода AM1 рассчитаны теплоты  
образования, теплоты тавтомеризации, дипольные моменты и верти-  
кальные потенциалы ионизации шестнадцати 2-, 4- и 5-замещенных  
азафосфолов в газовой фазе и в среде с высокой диэлектрической  
проницаемостью. Заместителями служили метильная, формоксильная  
и нитрогруппы. Влияние растворителя смоделировано методом само-  
согласованного реакционного поля. Найдено, что в газовой фазе и в  
среде с высокой диэлектрической проницаемостью главным тавтомер-  
ным компонентом исследованных соединений является NH-форма. В  
среде с низкой диэлектрической проницаемостью может присутство-  
вать и PH-тавтомер, который существенно влияет на общую реакцион-  
ную способность соединения.

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ASENDATUD AZAFOSFOOLIDE TAUTOMEERIA

Kuuestikümnelt 2-, 4- ja 5-asendatud azafosfoolide tautomeerilise  
AM1 tautomeerisatsioonivälja meetodi abil, arvutati soojusilmsed  
kvaliteetide, tautomeerisatsioonivälja, dipoolmomentide ja verti-  
kaalsete ionisatsioonipotentsiaalide arvutamiseks AM1-meetodi  
abil keskkonnas ning kõrge dielektrilise läbitavusega keskkonnas. Ase-  
ndajateks kasutati metüül-, formoksi- ja nitrogruppi. Lahusti-  
dumõju mõju modelleeriti kooskõlalise reaktsioonivälja meetodi abil.