Simulation of Reactive channels for Inorganic Cycle SNP2 Formation: A Study via *ab Initio* Molecular Dynamics

COUTINHO,N.D.C[1,*](PG), OLIVEIRA,H.C.B[1] (PQ), CARVALHO, V.H.[2] (PQ)

[1] *Instituto de Química, Universidade de Brasília, 70904-970, Brasília, Brasil.*
[2]*Grupo de Química Teórica e Estrutural de Anápolis, Campus de Ciências Exatas e Tecnológicas, Universidade Estadual de Goiás, 75001-970, Anápolis, Brasil)*
**nayaradcoutinho@gmail.com*

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INTRODUCTION

Inorganic heterocyclics have aroused great interest in synthetic and computational chemistry in recent years.[12] Recently, Zeng and coauthors synthesized a new aromatic ring compound (cycle SNPNP) through the pyrolysis of $SP(N_3)_3$.[3] In order to understand the formation of this compound, the authors conducted electronic structure calculations indicating the formation of the cycle by dimerization of the SNP and subsequent elimination of a sulfur atom from a six-membered ring (SNPSNP).

In order to get a full description of the mechanism of formation of the cycle-SNPNP, this work proposes to perform a Born-Oppenheimer molecular dynamics, aiming to check the mechanism already proposed and propose other possibilities for cycle formation.

METHODS

The Born-Oppenheimer molecular dynamics simulations were performed using the Gaussian 09 program. First, we used the semiempirical PM6 method. Subsequently, in order to obtain a better description of the energy and make it possible to compare the results obtained by Zeng and coauthors[3], we employed the B3LYP/6-311+G(3df) level of calculation. All simulations were developed at 1000 °C, which is the experimental temperature used in the synthesis.

RESULTS AND DISCUSSION

The Born-Oppenheimer molecular dynamics simulations were able to confirm the mechanism proposed by Zeng and coworkers. At 0.50 ps, it was possible to verify the formation of the six-membered cycle. For about 0.50 ps, this compound undergoes several structural conformations, and close to 1.052 ps the release of a sulfur atom and subsequent formation of the five-membered aromatic ring was observed, as can be seen in Figure 1a.

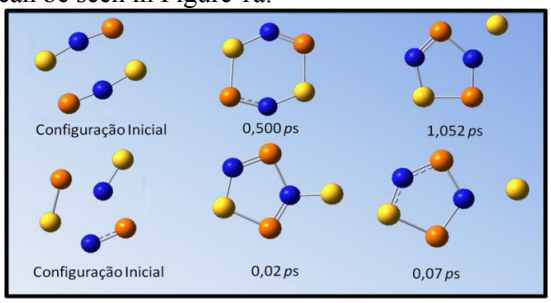

Figure 1. Simulation cycle-SNPNP formation (a) from the dimerization of the SNP and (b) from the reaction between the molecules NP, NS, PS using Born-Oppenheimer molecular dynamics with the semiempirical PM6 method.

Furthermore, calculations were performed to elucidate other possible mechanisms of cycle-SNPNP formation from the other products formed in the pyrolysis of $SP(N_3)_3$, such as: NP, NS, HN3 and PS. These simulations show that the cycle-SNPNP can also be formed from the reaction between NP, NS and PS, as shown in Figure 1b. The calculations using the B3LYP/6-311+G(3df) level are nearing completion.

CONCLUSION

The Born-Oppenheimer molecular dynamics simulations showed two possible mechanisms for cycle-SNPNP formation from the products of pyrolysis $SP(N_3)_3$: the first one is formed from SNP dimerization and subsequent elimination of the sulfur atom; the second one is formed by linking NP, NS and PS.

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