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1,2-Phosphorus Migrations in N-Phosphorylated N-heterocyclic carbenes

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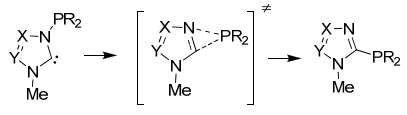

1 **2** **3**

X,Y=CR,N;
R=t-Bu; NMe_2; $N(i\text{-}Pr)_2$

Theoretical studies on stable N-phosphorylated N-heterocyclic carbenes showed that the main thermal transformation pathway for them was the migration of phosphorus to the carbene center yielding C-phosphorylated azoles (**3**). A mechanism of such rearrangement remained unclear.

We have carried out DFT calculations covering several possible routes for this migration in model NHCs **1**. The results show that the most plausible pathway is the thermal rearrangement of isolated carbenes by the intramolecular route via three-center transition state structures. Intermolecular mechanism of the rearrangement cannot be excluded in case during synthesis of carbenes.