

# QUANTUM CHEMICAL STUDY OF STRUCTURAL CHANGES OF SOME TRIAZENES, AZO-COMPOUNDS

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Balancing geometry of triazenes molecules  $R-C_6H_4-NH-N=N-C_6H_4-NO_2$  (where  $R = H, p-CH_3, o-CH_3, m-CH_3, p-Cl,$  and  $p-Br$ ) and their isomeric forms  $R-C_6H_4-N=N-NH-C_6H_4-NO_2$  were studied in this work by non-empiric method of Hartree-Fock-Roothaan with use of program GAMESS and basic set 3-21G\*\*. It was estimated that iso-form in gas phase is more advantageous energetically

## *Triazenes and their iso-forms in vacuum*

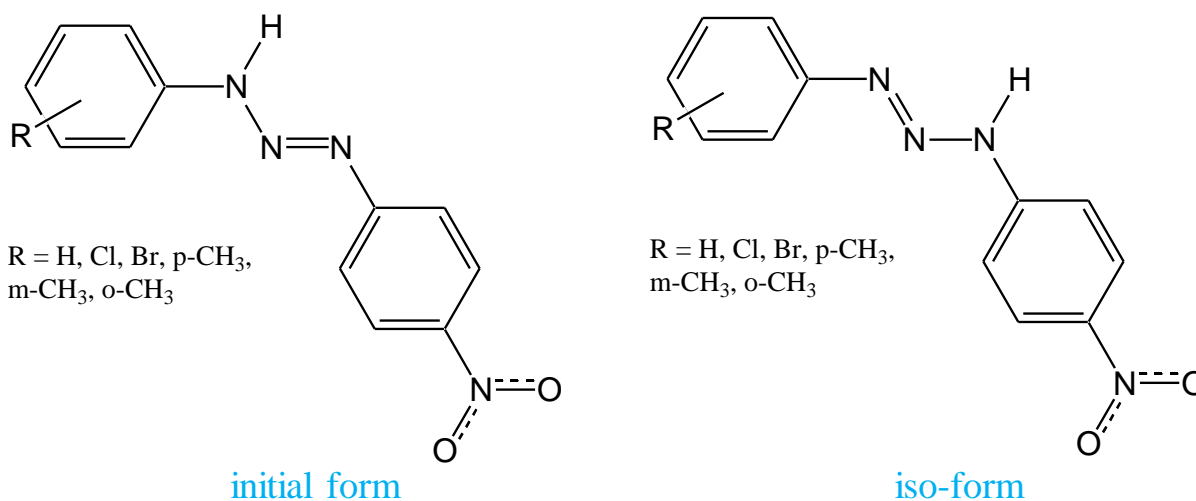


Table. Total energies of triazene molecules studied (a.u.)

Structure	Initial form	Iso-form
H-compound	-822.96122	-822.96521
p-CH <sub>3</sub> -substitution	-861.79117	-861.79605
m-CH <sub>3</sub> -substitution	-861.79198	-861.79565
o-CH <sub>3</sub> -substitution	-861.78506	-861.79163
p-Cl-substitution	-1279.77631	-1279.78007
p-Br-substitution	-3382.64372	-3382.64747
p-NO <sub>2</sub> -substitution	-1025.24972	

## Conclusions

Thus, the results of quantum-chemical calculations support the proposed mechanism of re-diazotating of triazenes and describe the observed influence of nature of the solvents and substituents in azo-component. Our results suggest, the process of interaction of diazonium cation with triazene should be regarded by taking into account the interaction of the solvent with both reactants.