

Showcasing research from University of Coimbra, Portugal; Université de Pau et des Pays de l'Adour, France; and The University of Queensland, Brisbane, Australia

Bond-shift isomers: the co-existence of allenic and propargylic phenylnitrile imines

Photolysis of matrix-isolated 5-phenyltetrazole generates two forms of phenylnitrile imine: propargylic and allenic. They are not resonance structures but correspond to different energy minima, representing bond-shift isomers. Upon further photolysis both of them convert into 1*H* diazirine. This is the first observation of bond-shift isomers for a 1,3-dipolar species (phenylnitrile imine) and one of the few observations of antiaromatic 1*H* diazirines.



