Prototropic Rearrangement of 2-Propynyl(methyl)amino, 2-Propynyloxy, and 2-Propynylsulfanyl Derivatives of Hetarenes under Conditions of Phase-Transfer Catalysis: Mechanism and Limitations

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Abstract—2-Propynyl derivatives of *N*-methylaniline, phenol, benzenethiol, 2-pyridinethiol, 2-pyrimidinethiol, and 1,3-benzoxazole-2-thiol were synthesized. Under conditions of phase-transfer catalysis, phenyl 2-propynyl sulfide is converted into allenyl phenyl sulfide and phenyl 1-propynyl sulfide. The rearrangement mechanism was studied by the AM1 quantum-chemical method.