Erratum to: Theoretical and experimental study of the regioselectivity of phenylacetylene 1,3-dipolar cycloaddition to some arylazides

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The original article has been published incorrectly with an error in the first and second paragraphs on page 4 and Table 2. The correct version is given below:

Spectral data for products

4-Phenyl-1-(2,4,6-trichlorophenyl)-1H-1,2,3-triazole (4)

White solid; yield: 79 %; mp = 115–117 °C (Anal. Calcd for C₁₄H₈Cl₃N₃: C, 51.80; H, 2.48; N, 12.95. Found: C, 51.25; H, 2.32; N, 12.77.); IR (KBr): 3,127, 3,051 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ = 7.972 (1H, s), 7.51 (2H, m), 7.40 (3H, m), 7.28 (2H, m); MS, *m/z* = 324 (M⁺).

5-Phenyl-1-(2,4,6-trichlorophenyl)-1H-1,2,3-triazole (5)

Light brown solid; yield: 21 %; mp = 126–128 °C (Anal. Calcd for C₁₄H₈Cl₃N₃: C, 51.80; H, 2.48; N, 12.95. Found: C, 51.84; H, 2.37; N, 12.13.); IR (KBr): 3,127, 3,033 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ = 7.975 (1H, s), 7.96 (2H, m), 7.59 (2H, s), 7.51 (2H, m), 7.42 (1H, m); MS, *m/z* = 324 (M⁺).

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Table 2 Energies of reactants, transition states and cycloadducts **4**, **5**, **8**, **9**, **12**, and **13** E (a.u.), relative activation energies ΔE_a (kcal mol⁻¹), and energy differences between products and reactants, ΔE_r (kcal mol⁻¹)

Reactions	System	<i>E</i>	ΔE_a^a	ΔE_r^a
1	Arylazide 2	-1774.781		
	Phenylacetylene 3	-308.462		
	TS 4	-2083.214	18.2	
	TS 5	-2083.205	23.8	
	4	-2083.337		-58.7
	5	-2083.333		-56.1
2	Arylazide 7	-639.812		
	Phenylacetylene 3	-308.462		
	TS 8	-948.251	14.3	
	TS 9	-948.239	21.8	
	8	-948.364		-56.4
	9	-948.360		-54.1
3	Arylazide 11	-600.484		
	Phenylacetylene 3	-308.462		
	TS 12	-908.916	18.2	
	TS 13	-908.902	27.3	
	12	-909.041		-60.1
	13	-909.034		-55.8

^a To reactants