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Diphosphonylation of Aromatic Diazaheterocycles and Theoretical Rationalization of Product Yields

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Keywords: Phosphonylation / Nitrogen heterocycles / Nucleophilic addition / Density functional calculations

In the original article,[1] *compounds* ***5a–c*** *in Figure 2 (p. 1059) and in Table 1 (p. 1060) each lack a bond in the phenanthroline core. The correct Figure 2 and Table 1 are depicted below.*

The Authors

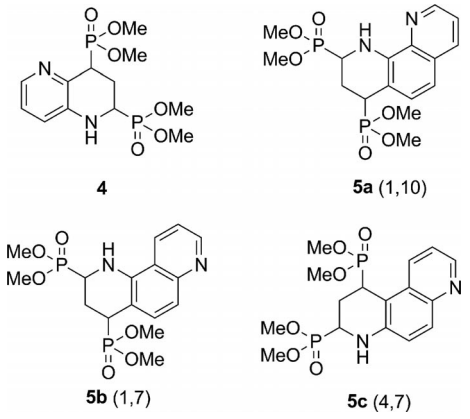

Figure 2. Diphosphonylated 1,5-naphthyridine **4** and phenanthrolines **5a–c**.

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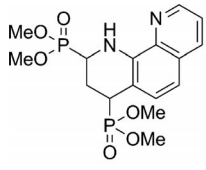
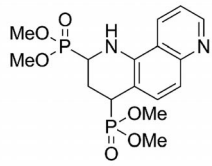
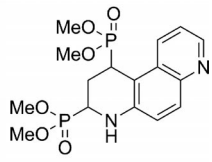
Table 1. Reaction of different phenanthrolines **5** with dimethyl trimethylsilyl phosphite (DMPTMS) in acidic medium.[a]



5a (1,10)



5b (1,7)



5c (4,7)

Entry	Product **5**	Equiv. DMPTMS	Equiv. H_2SO_4	Time		Conversion [%]		Isolated yield [%]		Ratio M/*m*
				Δ [d]	MW [h]	Δ	MW	Δ	MW	
1	1,10-	2.05	0.5	5	–	1	–	–	–	–
2	1,7-	2.05	0.5	3	–	0	–	–	–	–
3	4,7-	2.05	0.5	6	–	14	–	–	–	–
4	4,7	4	1	1	–	1	–	–	–	–
5	1,10-	6	1	–	2	–	95	–	88	93:7
6	1,10-	3	0.5	–	3	–	86	–	75	92:8
7	1,10-	3.5	0.5	–	5	–	100	–	96	94:6
8	1,10-	3 × 1	0.5	–	5	–	62	–	48	95:5
9	1,10-	3 × 2	3 × 0.4	–	5	–	26	–	–	–
10	1,7-	3	0.5	–	5	–	67	–	25	>99:1
11	1,7-	3 × 1	1	–	5	–	35	–	12	98:2
12	1,7-	3 × 2	3 × 0.4	–	5	–	20	–	–	–
13	4,7-	6	1	–	3	–	36	–	12	91:9
14	4,7-	3 × 2	1	–	5	–	22	–	8	90:10
15	4,7-	3 × 2	3 × 0.4	–	5	–	15	–	–	–

[a] Δ = reflux, batch; MW = microwave heating (45 °C, 200 W), m = minor diastereomeric pair; M = major diastereomeric pair.

[1] A. De Blieck, S. Catak, W. Debrouwer, J. Drabowicz, K. Hemelsoet, T. Verstraelen, M. Waroquier, V. Van Speybroeck, C. V. Stevens, *Eur. J. Org. Chem.* **2013**, 1058–1067

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