

# ADDITIONS AND CORRECTIONS

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Sergey I. Druzhinin, Sergey Kovalenko,\* Tamara A. Senyushkina, Attila Demeter, Reinhard Machinek, Mathias Noltemeyer, and Klaas A. Zachariasse\*: Intramolecular Charge Transfer with the Planarized 4-Cyanofluorazene and Its Flexible Counterpart 4-Cyano-*N*-phenylpyrrole. Picosecond Fluorescence Decays and Femtosecond Excited-State Absorption

Page 8240. In Table 1, errors have occurred in the entries for the angles C(1)–N(7)–C(8), C(1)–N(7)–C(11) and C(8)–N(7)–C(11) of FPP4C exp and FPP calc. Further, due to a change in the table caption, several superscripts at data for these angles, as well as for the pyramidal angle  $\varphi$  became incorrect. The conclusions of the paper are not affected.

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**TABLE 1: Data for the Ground-State Structure of FPP4C, PP4C, FPP and PP from X-ray Crystal Analysis (exp) and from Calculations (calc)<sup>a</sup>**

	FPP4C exp	PP4C exp <sup>b</sup>	PP4C exp <sup>c</sup>	PP4C calc <sup>e</sup>	FPP calc <sup>d,e</sup>	FPP calc <sup>f,g</sup>	PP exp <sup>h</sup>	PP calc <sup>d,e,i</sup>	PP calc <sup>f,g,i</sup>
N(7)–C(1)	139.9	140.7	140.6	141.0	139.7	139.6	142.3	141.3	141.5
N(7)–C(8)	138.5	137.9	138.2	138.9	136.8	136.6	137.9	137.5	137.3
N(7)–C(11)	138.2	137.9	138.2	138.9	137.4	137.0	137.9	137.5	137.3
C(1)–C(2)	139.8	139.4	139.0	140.6	140.5	138.1	139.4	139.8	139.6
C(1)–C(6)	138.4	139.4	139.0	140.6	138.5	138.1	139.4	139.8	139.2
C(2)–C(3)	138.1	138.5	138.8	139.1	138.5	138.1	138.9	139.5	139.1
C(3)–C(4)	140.6	139.6	138.9	139.1	140.5	140.1	138.8	139.5	139.1
C(4)–C(5)	140.0	139.6	138.9	140.7	139.3	139.6	138.8	139.5	139.2
C(5)–C(6)	139.3	138.5	138.8	140.7	140.3	139.9	138.9	139.5	139.6
C(8)–C(9)	136.7	137.0	135.5	137.6	137.3	137.4	136.2	136.9	137.1
C(9)–C(10)	142.3	140.8	141.1	143.0	143.7	143.7	141.2	142.9	143.2
C(10)–C(11)	135.9	137.0	135.5	137.6	136.8	136.8	136.2	136.9	137.1
C(11)–C(12)	150.8				150.9	151.0			
C(2)–C(12)	152.2				152.3	152.3			
C(4)–C(13)	144.1	143.2	144.6	143.5					
C(13)–N(14)	115.0	114.7	111.6	116.5					
C(1)–N(7)–C(8)	137.9	125.7	126.2	125.8	138.2 <sup>e</sup>	138.1 <sup>g</sup>	126.3	125.8 <sup>e</sup>	125.7 <sup>g</sup>
C(1)–N(7)–C(11)	112.0	125.7	126.2	125.8	111.7 <sup>e</sup>	111.7 <sup>g</sup>	125.8	125.8 <sup>e</sup>	125.6 <sup>g</sup>
C(8)–N(7)–C(11)	110.1	108.6	107.5	108.5	110.1 <sup>e</sup>	110.3 <sup>g</sup>	107.9	108.4 <sup>e</sup>	108.7 <sup>g</sup>
$\sum N^j$	360.0	360.0	360	360	360	360	360.0	360.0	360
twist angle $\theta^k$	1.0	24.2	24.0	30.9	0	0	5.7	42.7	39.4
pyramidal angle $\varphi^l$	0.2	0.0	0.0	0.0	0.0 <sup>e</sup>	0.1 <sup>g</sup>	0.3	0.0 <sup>e</sup>	0.1 <sup>g</sup>
quinoidality <sup>m</sup>	0.995	0.992	0.999	1.000	1.007	1.002	1.001	1.000	1.003

<sup>a</sup> See atom numbering in Chart 1 and Figure 1. The bond lengths are in picometers (pm), the angles are in degrees. <sup>b</sup> Data from ref 36. <sup>c</sup> Data from ref 37 (calc: DFT). <sup>d</sup> Data from ref 27 (CASSCF). <sup>e</sup> Private communication from ref 27. <sup>f</sup> Data from ref 28 (CASSCF). <sup>g</sup> Private communication from ref 28. <sup>h</sup> Data from ref 20. <sup>i</sup> For earlier computations, see ref 20. <sup>j</sup> Sum of the angles around the pyrrole nitrogen (Figure 1). <sup>k</sup> Twist angle  $\theta$ : (C(6)C(1)N(7)C(8) + C(6)C(1)N(7)C(11))/2 (Figure 1). <sup>l</sup> Pyramidal angle  $\varphi$ : angle between the vector N(7)C(1) and the plane C(8)N(7)C(11) (Figure 1). <sup>m</sup> Quinoidality: (C(5)–C(6))/(C(4)–C(5)) (Figure 1).