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Addition/Correction

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Correction to "Ultrafast Intramolecular Charge Transfer with Strongly Twisted Aminobenzonitriles: 4-(Di-*tert*-butylamino)benzonitrile and 3-(Di-*tert*-butylamino)benzonitrile"

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In Table 1, errors have occurred in the notation for the bond length data of MMD and DMABN: C(3)−C(4), C(4)−C(5), and C(5)−C(6). Further, in column 6 for NTC6, C(1)−C(13) has to be replaced by C(5)−C(6). In addition, there were typographical errors in the heading of the table. The conclusions of the paper are not affected. We also provide updated information for ref 47 from the original paper as ref 1 below.

REFERENCES

(1) Druzhinin, S. I.; Mayer, P.; Stalke, D.; von Bülow, R.; Noltemeyer, M.; Zachariasse, K. A. Intramolecular Charge Transfer with 1-*tert*-Butyl-6-cyano-1,2,3,4-tetrahydroquinoline (NTC6) and Other Aminobenzonitriles. A Comparison of Experimental Vapor Phase Spectra and Crystal Structures with Calculations. *J. Am. Chem. Soc.* **2008**, *132*, 7730−7744.

Table 1. Data for the Ground-State Structure of 3-(Di-*tert*-butylamino)benzonitrile (mDTABN), 3,5-Dimethyl-4-(dimethylamino)benzonitrile (MMD), 4-(Dimethylamino)benzonitrile (DMABN), and 1-*tert*-Butyl-6-cyano-1,2,3,4-tetrahydroquinoline (NTC6) from X-ray Crystal Analysis where the Bond Lengths are in pm (See the Molecular Structures in Chart A)

	mDTABN[a] (A)	mDTABN[a] (B)	MMD[b]	DMABN[c]		NTC6[d]
N(7)−C(X)[e]	143.7	143.8	141.4	136.5	N(1)−C(9)	137.4
N(7)−C(10)	150.5	150.2	144.1	144.8	N(1)−C(13)	149.3
N(7)−C(14)	150.4	151.1	144.1	144.8	N(1)−C(2)	147.6
C(1)−C(2)	139.7	139.8	138.7	138.8	C(5)−C(6)	140.0
C(1)−C(6)	139.0	138.5	138.7	138.8	C(6)−C(7)	139.1
C(1)−C(8)	144.2	144.4	142.5	142.7	C(6)−C(11)	143.3
C(2)−C(3)	138.9	138.8	138.2	137.0	C(5)−C(10)	137.9
C(3)−C(4)	139.6	139.6	140.8	140.0	C(9)−C(10)	142.1
C(4)−C(5)	138.6	139.2	140.8	140.0	C(8)−C(9)	141.0
C(5)−C(6)	137.6	138.0	138.2	137.0	C(7)−C(8)	137.8
C(8)−N(9)	114.3	114.5	114.7	114.5	C(11)−N(12)	115.0
C(10)−C(11)	153.4	153.4	–	–	C(13)−C(14)	153.9
C(10)−C(12)	153.0	153.4	–	–	C(13)−C(15)	152.9
C(10)−C(13)	152.6	152.9	–	–	C(13)−C(16)	153.2
C(14)−C(15)	153.0	153.0	–	–	C(2)−C(3)	151.3
C(14)−C(16)	154.1	153.1	–	–		–
C(14)−C(17)	153.8	153.9	–	–		–
C(X)−N(7)−C(10)[e]	112.2	113.0	118.3	121.5	C(2)−N(1)−C(9)	119.8
C(10)−N(7)−C(14)	123.2	123.5	116.2	116.4	C(2)−N(1)−C(13)	123.4
C(X)−N(7)−C(14)[e]	115.1	114.3	119.2	120.6	C(9)−N(1)−C(13)	115.8
twist angle θ^f	86.4	86.6	57.4	0.0	twist angle θ^g	22.7
$\sum N^h$	350.6	350.7	353.8	358.5	$\sum N^i$	359.0
pyramidal angle φ^j	32.5	32.2	24.4	12.1	pyramidal angle φ^k	9.6
quinoidality factor[l]	0.9910	0.9953	0.9964	0.9870	quinoidality factor[m]	0.9907

[a]Data (A) and (B) for two different molecules in the unit cell. The standard deviations are 0.2−0.3 pm for the bond lengths and 0.2° for the angles. [b]Reference 48, at 173 K. [c]Reference 48, at 253 K. [d]Reference 47 from the original paper (ref 1 below); see below. [e]X = 3 for mDTABN, X = 4 for the other molecules. [f]Twist angle: (C(3)C(4)N(7)C(10) + C(5)C(4)N(7)C(14))/2 for MMD and DMABN. [g]Twist angle: (C(8)C(9)N(1)C(13) + C(10)C(9)N(1)C(2))/2 for NTC6. [h]Sum of the angles around the amino nitrogen N(7). [i]Sum of the angles around the amino nitrogen N(1). [j]Pyramidal angle: angle between the vector N(7)−C(X) and the plane C(10)N(7)C(14). [k]Pyramidal angle: angle between the vector N(1)−C(9) and the plane C(2)N(1)C(13). [l]Quinoidality factor for the phenyl ring: (C(5)−C(6))/(C(1)−C(6)). [m]Quinoidality factor for the phenyl ring: (C(7)−C(8))/(C(6)−C(7)).

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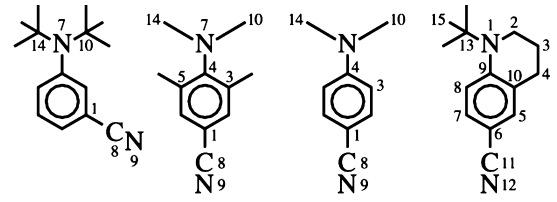
Chart A



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