Appendix A
Calculated Structural Parameters

See (Tables A.1 and A.2).

Table A.1 The coordinates and bond lengths of 3,5-dibromo-3′,5′-difluoro-4′-cyanobiphenyl, as calculated at density functional level of theory by colleagues at the University of Helsinki, according to the details presented in Refs. [1, 2]

Atom	Coordinates(Å)		
	x	y	z
N	0.00	0.00	7.03
C1	0.00	0.00	5.88
C2	0.00	0.00	4.46
C3	-0.99	-0.66	3.72
C4	-1.00	-0.67	2.34
C5	0.00	0.00	1.63
C6	1.00	0.67	2.34
C7	0.99	0.66	3.72
C8	0.00	0.00	0.15
C9	-1.20	0.11	-0.56
C10	-1.18	0.11	-1.95
C11	0.00	0.00	-2.66
C12	1.18	-0.11	-1.95
C13	1.20	-0.11	-0.56
F1	-1.94	-1.31	4.38
F2	1.94	1.31	4.38
Br1	-2.83	0.28	-2.90
Br2	2.83	-0.28	-2.90
H1	-1.78	-1.22	1.83
H2	1.78	1.22	1.83
H3	-2.14	0.22	-0.03
H4	2.14	-0.22	-0.03
H5	0.00	0.00	-3.74

Bond	Length (Å)
Br1-C10	1.91
Br2-C12	1.91
C10-C9	1.39
C11-C10	1.39
C12-C11	1.39
C13-C12	1.39
C13-C8	1.40
C2-C1	1.42
C3-C2	1.40
C4-C3	1.38
C5-C4	1.40
C6-C5	1.40
C7-C2	1.40
C7-C6	1.38
C8-C5	1.48
C9-C8	1.40
F1-C3	1.34
F2-C7	1.34
H1-C4	1.08
H2-C6	1.08
H3-C9	1.08
H4-C13	1.08
H5-C11	1.08
N-C1	1.15

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Table A.2 The bond angles of 3,5-dibromo-3′,5′-difluoro-4′-cyanobiphenyl, as calculated at density functional level of theory by colleagues at the University of Helsinki, according to the details presented in Refs. [1, 2]

Bond Pair	Angle (Degrees)
Br1-C10-C11	119.0
Br1-C10-C9	119.3
Br2-C12-C11	119.0
Br2-C12-C13	119.3
C10-C9-C8	119.7
C11-C10-C9	121.8
C12-C11-C10	117.9
C12-C13-C8	119.7
C13-C12-C11	121.8
C13-C8-C9	119.2
C1-C2-C3	121.9
C1-C2-C7	121.9
C2-C1-N23	180.0
C4-C3-C2	122.7
C5-C4-C3	119.7
C5-C8-C13	120.4
C5-C8-C9	120.4
C6-C5-C4	119.1
C6-C7-C2	122.7

Bond Pair	Angle (Degrees)
C7-C2-C3	116.2
C7-C6-C5	119.7
C8-C5-C4	120.4
C8-C5-C6	120.4
F1-C3-C2	118.2
F1-C3-C4	119.1
F2-C7-C2	118.2
F2-C7-C6	119.1
H1-C4-C3	118.7
H1-C4-C5	121.6
H2-C6-C5	121.6
H2-C6-C7	118.7
H3-C13-C8	120.4
H3-C9-C10	119.9
H3-C9-C8	120.4
H4-C13-C12	119.9
H5-C11-C10	121.1
H5-C11-C12	121.1

Dihedral Bond Linkage	Angle (Degrees)
C4-C5-C8-C9	39.0

References

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2. C.B. Madsen, L.B. Madsen, S.S. Viftrup, M.P. Johansson, T.B. Poulsen, L. Holmegaard, V. Kumarappan, K.A. Jorgensen, H. Stapelfeldt, J. Chem. Phys. **130**, 234310 (2009)