Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Pressure-preferred symmetric reactions of 4,4'-bipyridine hydrobromide

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Table S1. Comparison of CH···Br contacts in the structure of 44'biPy2CH_3Br calculated for the methyl-group orientation obtained by using constrains AFIX 33 and AFIX 137. Because the H···Br contacts are shorter for the AFIX 33 constrain, this model has been accepted for the discussions in the text.

44'biPy2CH_3Br						
	AFIX 33			**AFIX 137**		
CH···Br	H···Br (Å)	C···Br (Å)	C-H···Br (°)	H···Br (Å)	C···Br (Å)	C-H···Br (°)
C6-H6···Br^{j}	2.793	3.664(22)	156	2.794	3.668(21)	157
C2-H2···Br^{ij}	2.830	3.592(18)	140	2.825	3.589(18)	140
C3-H3···Br^{jj}	2.770	3.662(20)	161	2.772	3.663(20)	161
C7-H7b···Br^{ij}	3.036	3.795(26)	137	3.212	3.792(26)	121
C7-H7c···Br^{jv}	2.955	3.722(25)	138	3.029	3.713(24)	129

Table S2. Crystal data and structure-refinements details for 44'biPy2HBr.

Pressure	0.10(2) MPa	0.10(2) GPa	0.20 (2) GPa	0.50(2) GPa	1.00(2) GPa
Temperature (K)	296(2)	296(2)	296(2)	296(2)	296(2)
Formula weight	318.02	318.02	318.02	318.02	318.02
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
Unit cell dimensions (Å,°)					
a	4.8986(6)	4.8839(15)	4.874(4)	4.8450(11)	4.8011(17)
b	7.6614(10)	7.622(5)	7.567(6)	7.453(2)	7.275(4)
c	7.9890(9)	7.951(4)	7.936(4)	7.875(5)	7.759(5)
α	70.464(11)	70.87(6)	70.73(6)	70.89(4)	71.06(6)
β	87.005(10)	86.78(4)	86.64(5)	86.82(4)	86.46(5)
γ	77.176(11)	77.39(5)	77.47(7)	77.82(2)	78.64(4)
Volume ($Å^3$)	275.44(6)	272.8(3)	269.7(3)	262.61(19)	251.3(2)
Z	1	1	1	1	1
Calculated density (g/cm^3)	1.917	1.935	1.958	2.011	2.101
Absorption coefficient (mm^{-1})	0.408	7.389	7.476	7.677	8.022
F(000)	154	154	154	154	154
Crystal size (mm)	0.30/0.15/0.12	0.24/0.12/0.11	0.21/0.16/0.11	0.26/0.11/0.10	0.26/0.11/0.10
θ-range for data collection (°)	4.27 to 25.29	2.71 to 27.71	4.65 to 27.20	4.30 to 26.44	4.33 to 34.93
Min/max indices:h, k, l	-5/5, -9/9, -9/9	-6/6, -2/2, -8/8	-6/6, -4/4, -9/9	-6/6,-9/9, -3/3	-7/7,-11/11, -4/4
Reflect. Collected/unique	3434 / 905	1219 / 183	1159 / 185	953 / 155	1865/309
R_{int}	0.0219	0.1986	0.0953	0.0487	0.0942
Refinement method	Full-matrix least-squares on F^2				
Completeness (%)	90.7	14.2	15.3	14.5	14.0
Data/restrains/parameters	905/0/64	183/0/ 22	185/6/34	155/6/34	309/0/34
Goodness-of-fit on F^2	1.045	1.211	1.048	1.438	1.006
Final R_1/wR_2 ($I>2\sigma_1$)	0.0184/0.0448	0.0623/0.1467	0.0487/0.1178	0.0332/0.0656	0.0511/0.1094
R_1/wR_2 (all data)	0.0193/0.0451	0.0670/0.1523	0.0535/0.1238	0.0427/0.0693	0.0820/0.1273

Table S3. Crystal data and structure-refinements details for 44'biPy2CH_3Br.

Pressure	0.35(2) GPa
Temperature (K)	296(2)
Formula weight	318.02
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions (Å,°)	
a	5.947(3)
b	8.068(8)
c	13.411(5)
α	90
β	95.94(3)
γ	90
Volume (Å^3)	640.0(7)
Z	2
Calculated density (g/cm^3)	1.796
Absorption coefficient (mm^{-1})	6.308
F(000)	340
Crystal size (mm)	0.28/0.22/0.15
θ-range for data collection (°)	3.05 to 27.23
Min/max indices:h, k, l	-7/7, -4/4, -16/16
Reflect. Collected/unique	2131/313
R_{int}	0.2281
Refinement method	Full-matrix least-squares on F^2
Completeness (%)	21.8
Data/restrains/parameters	313/0/33
Goodness-of-fit on F^2	1.041
Final R_1/wR_2 ($I>2\sigma_1$)	0.0879/0.2298
R_1/wR_2 (all data)	0.0970/0.2400

Table S4. Symmetry codes used for the shortest contacts in 44'biPy2HBr and 44'biPy2CH_3Br.

Code	Symmetry code	Code	Symmetry code
44'biPy2HBr		**44'biPy2CH_3Br**	
i	1+x, y, z	j	1+x, y, z
ii	1-x, 1-y, 2-z	jj	1+x, 0.5-y, 0.5+z
iii	x, 1+y, z	jjj	x, 0.5-y, 0.5+z
iv	1-x, 1-y, 1-z	jv	1-x, 1-y,1- z

Table S5. The shortest NH···Br and CH···Br contacts in 44'biPy2HBr and 44'biPy2CH_3Br.

DH···A	H···A (Å)	D···A (Å)	DH···A (°)
44'biPy2HBr			
0.1 MPa			
NH···Br			
N1-H1···Br1^{i}	2.447	3.207(2)	148
CH···Br			
C2-H2···Br1^{ii}	2.805	3.523(3)	135
C3-H3···Br1^{iii}	3.042	3.621(2)	122
C6-H6··· Br1^{iv}	2.896	3.616(3)	135
0.1 GPa			
NH···Br			
N1-H1···Br1^{i}	2.387	3.148(23)	148
CH···Br			
C2-H2···Br1^{ii}	2.810	3.522(15)	134
C3-H3···Br1^{iii}	3.002	3.598(42)	123
C6-H6··· Br1^{iv}	2.804	3.514(21)	134
0.2 GPa			
NH···Br			
N1-H1···Br1^{i}	2.572	3.276(44)	140
CH···Br			
C2-H2···Br1^{ii}	2.834	3.511(14)	130
C3-H3···Br1^{iii}	2.993	3.524(57)	118
C6-H6··· Br1^{iv}	2.876	3.528(33)	128
0.5 GPa			
NH···Br			
N1-H1···Br1^{i}	2.464	3.190(19)	142
CH···Br			
C2-H2···Br1^{ii}	2.751	3.419(53)	130
C3-H3···Br1^{iii}	3.013	3.518(22)	116
C6-H6··· Br1^{iv}	2.886	3.578(56)	132
1.0 GPa			
NH···Br			
N1-H1···Br1^{i}	2.481	3.184(17)	139
CH···Br			
C2-H2···Br1^{ii}	2.840	3.469(43)	126
C3-H3···Br1^{iii}	2.897	3.438(18)	118
C6-H6··· Br1^{iv}	2.796	3.531(44)	137
44'biPy2CH_3Br			
0.35 GPa			
CH···Br			
C6-H6···Br^{j}	2.793	3.664(22)	156
C2-H2···Br^{jj}	2.830	3.592(18)	140
C3-H3···Br^{jjj}	2.770	3.662(20)	161
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