

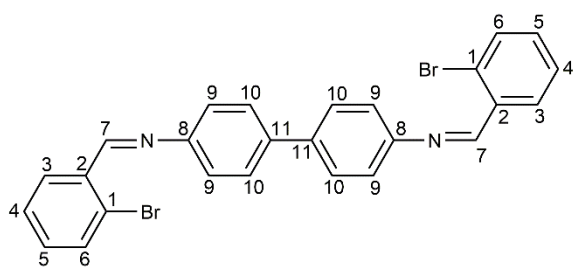
Electronic Supplementary Information

STRUCTURAL CHARACTERIZATION OF SOME SYMMETRIC BIS-IMINES

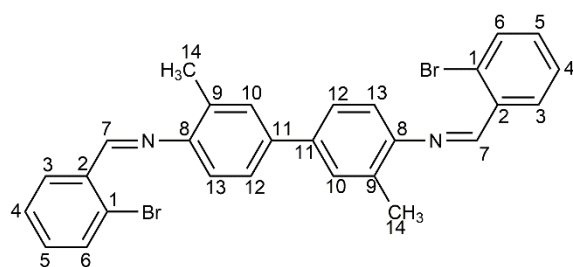
Adrian-Alexandru Someșan, Ioana Barbul, Richard A. Varga*

Department of Chemistry, Supramolecular Organic and Organometallic Chemistry Centre (SOOMCC),
Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, 11 Arany Janos, 400028 Cluj-
Napoca, Romania. E-mail: richard.varga@ubbcluj.ro.

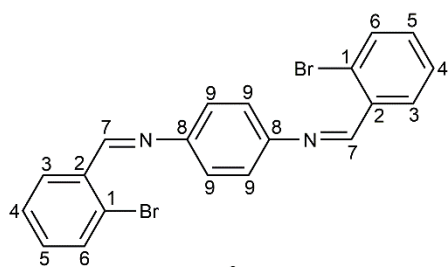
Numbering schemes for NMR resonance assignments



1



2



3

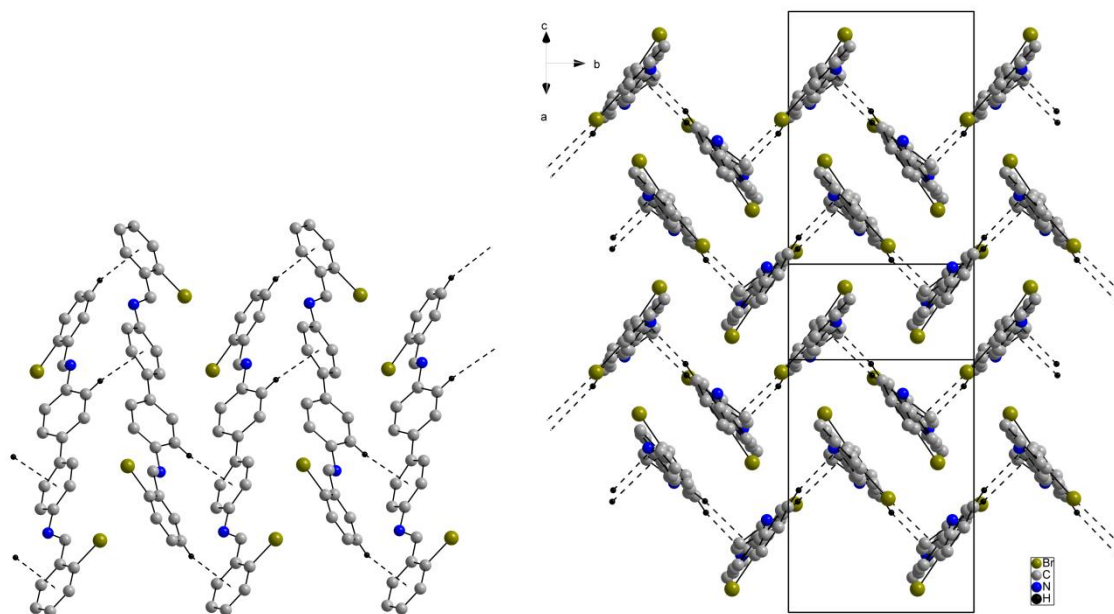


Figure S1. View of the zig-zag ribbon-like arrangement based on intermolecular C–H··· π interactions and the crystal packing of **1b** (only hydrogen atoms involved in the interactions are shown).

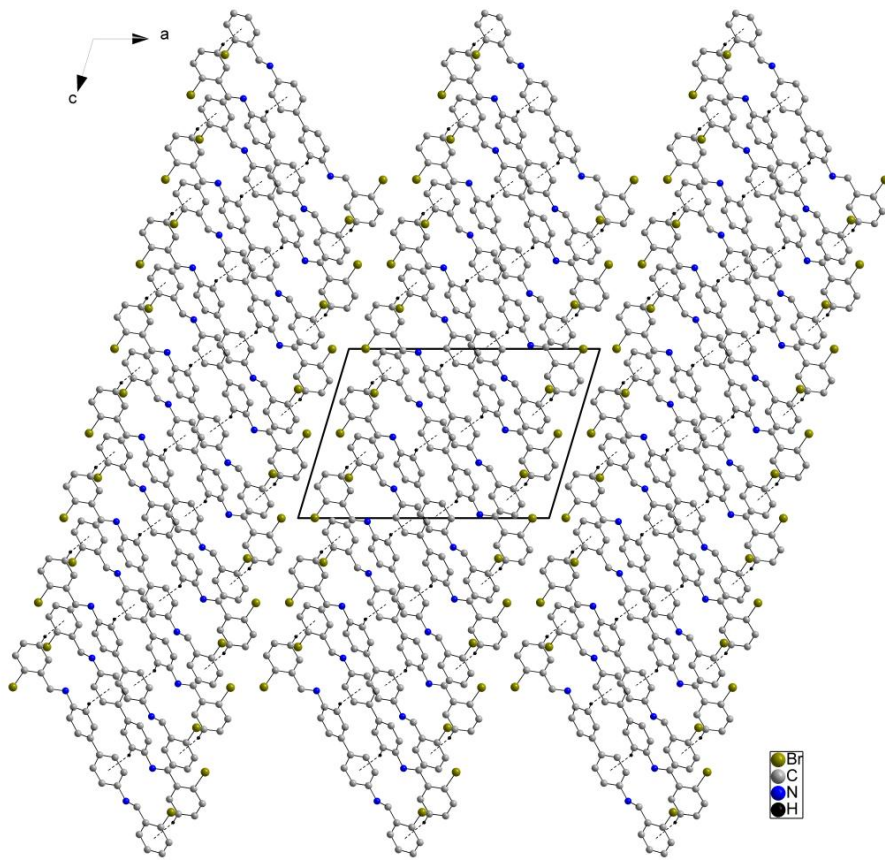
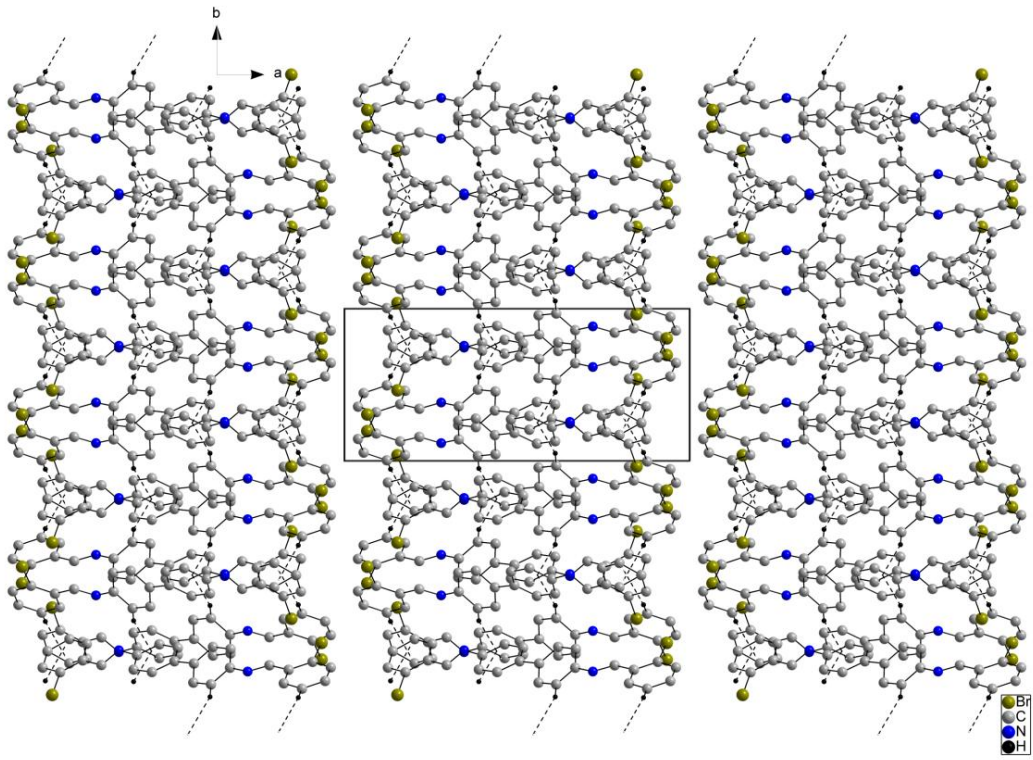


Figure S2. View along *c* and *b* axis of the crystal packing in **1b** showing the stacking of the ribbon-like arrangements based on intermolecular C–H··· π interactions (only hydrogen atoms involved in the interactions are shown).

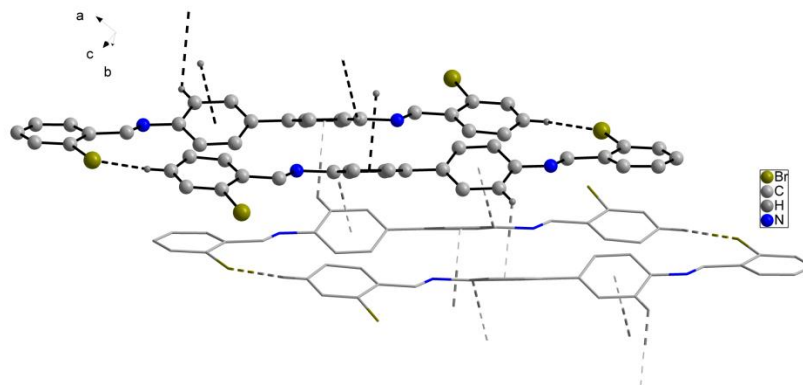


Figure S3. View of the intermolecular Br···H and C–H··· π interactions in the crystal of **1c** (only hydrogen atoms involved in the interactions are shown).

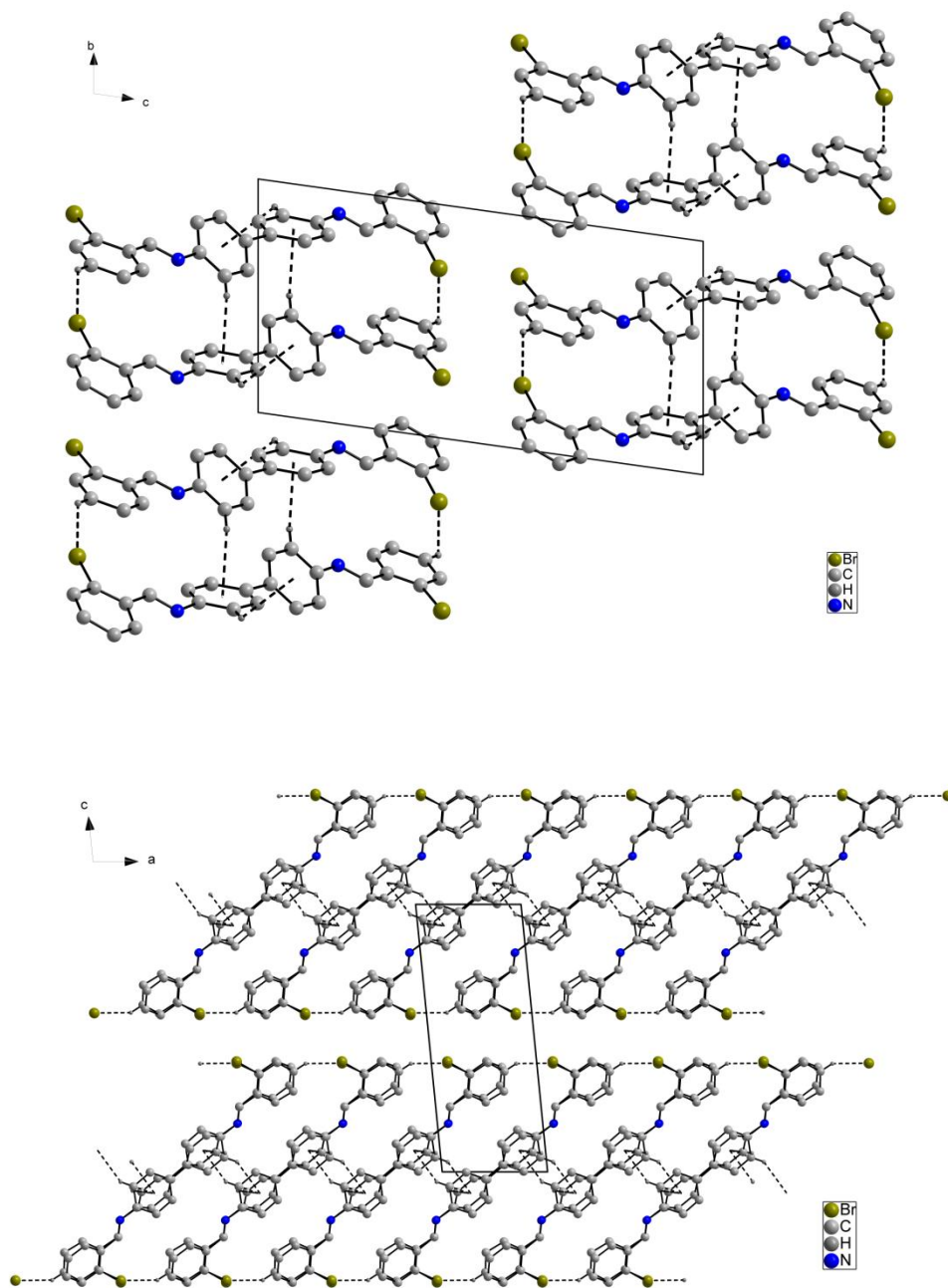


Figure S4. View along *a* and *b* axis of the crystal packing in **1c** showing the stacking of the ribbon-like arrangements based on C–H... π and Br...H intermolecular interactions (only hydrogen atoms involved in the interactions are shown).

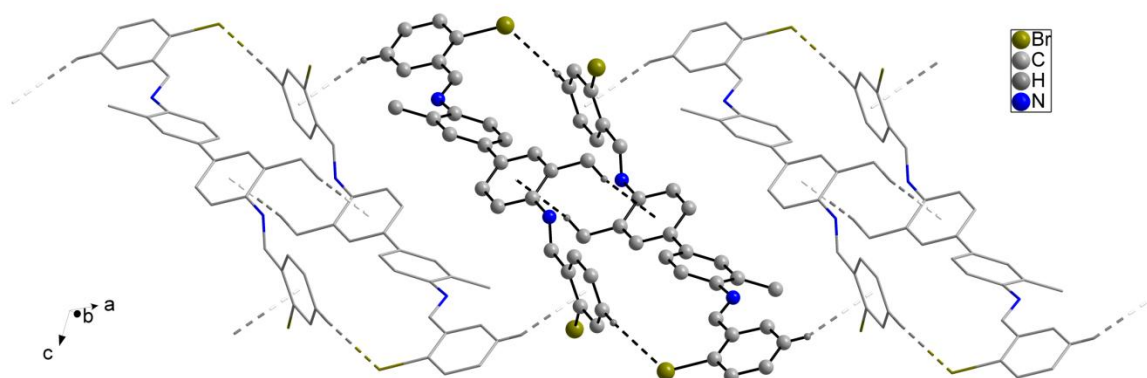


Figure S5. View of the intermolecular Br \cdots H and C–H \cdots π interactions in the crystal of **2** (only hydrogen atoms involved in the interactions are shown).

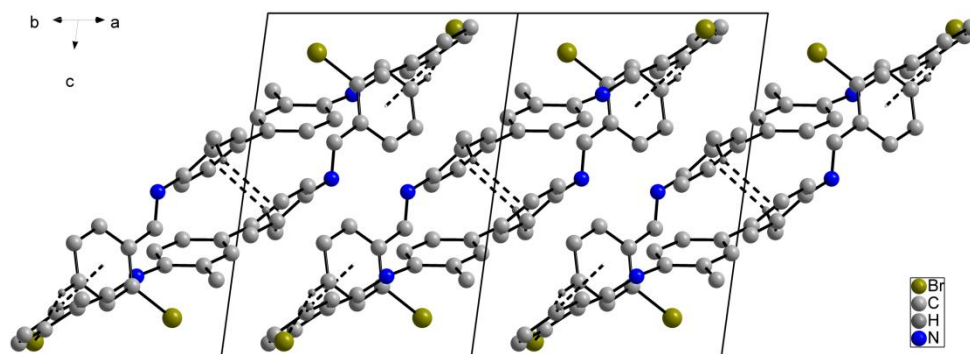


Figure S6. View of the crystal packing in **2** showing the stacking of the ribbon-like arrangements based on C–H \cdots π and Br \cdots H intermolecular interactions (only hydrogen atoms involved in the interactions are shown).

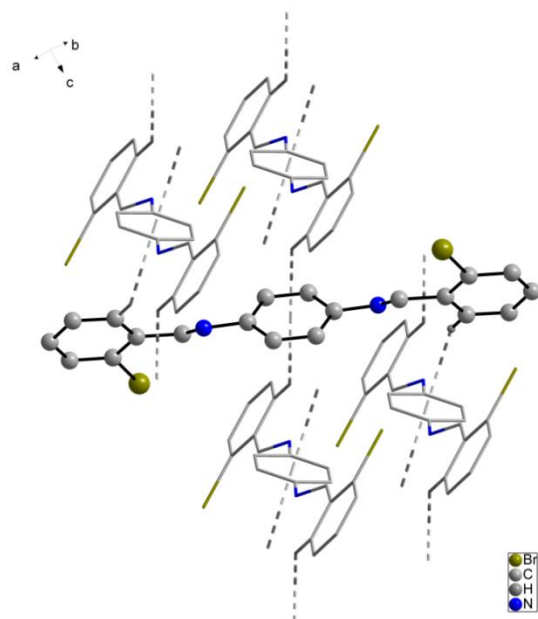


Figure S7. View of the intermolecular C–H··· π interactions in the crystal of **3** (only hydrogen atoms involved in the interactions are shown).

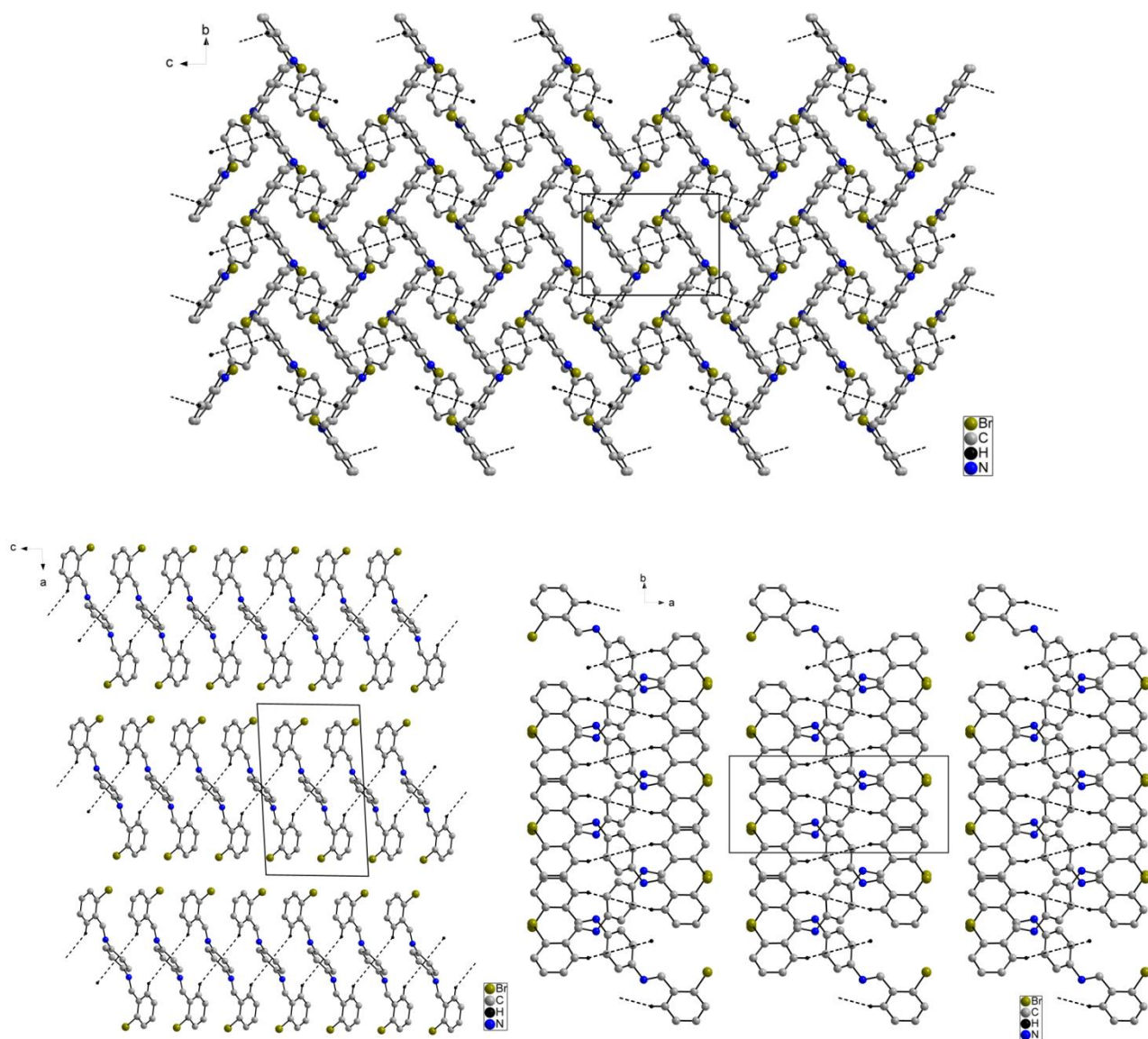


Figure S8. View of the crystal packing in **3** showing the layer-like arrangements based on C–H... π intermolecular interactions along the three axes (only hydrogen atoms involved in the interactions are shown).

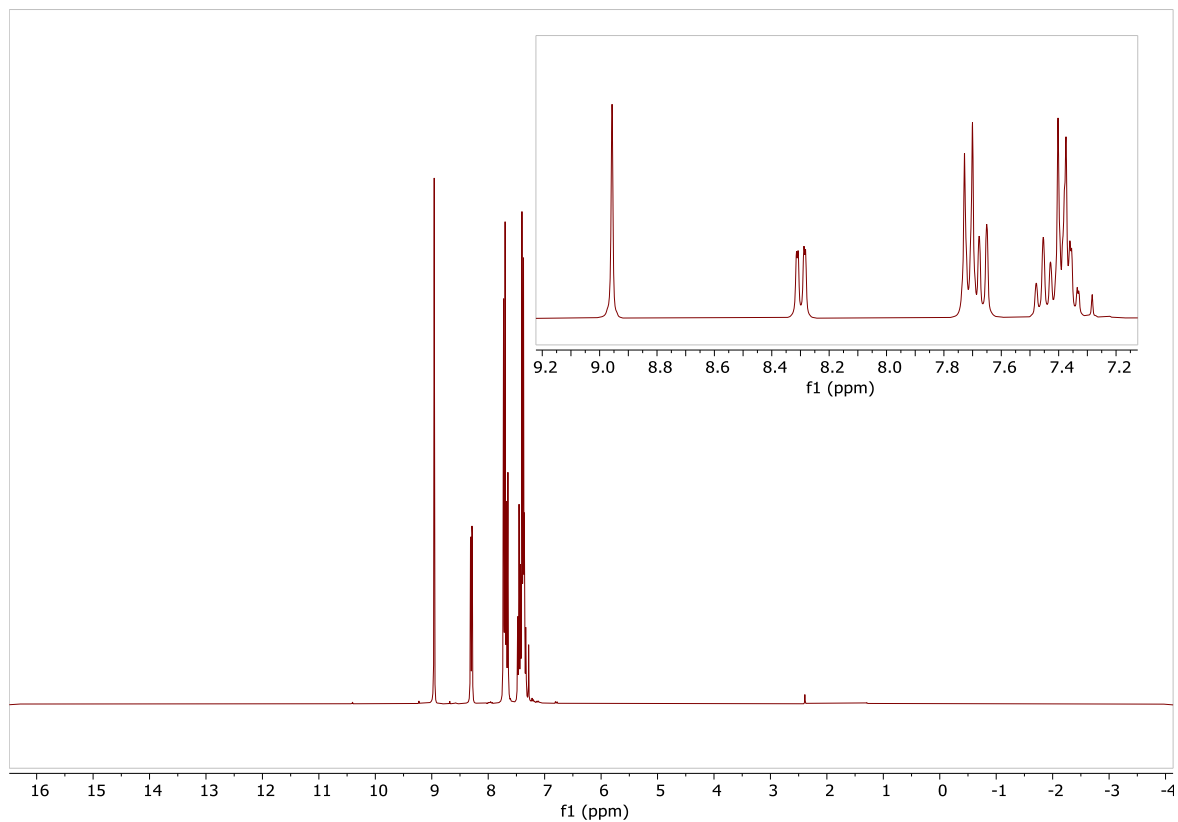


Figure S9. ^1H NMR (CDCl_3 , 20 °C) spectrum of $[1,1'-\{4,4'-[(2-\text{BrC}_6\text{H}_4)\text{CH}=\text{N}]_2\text{C}_6\text{H}_4\}]_2$ (**1**).

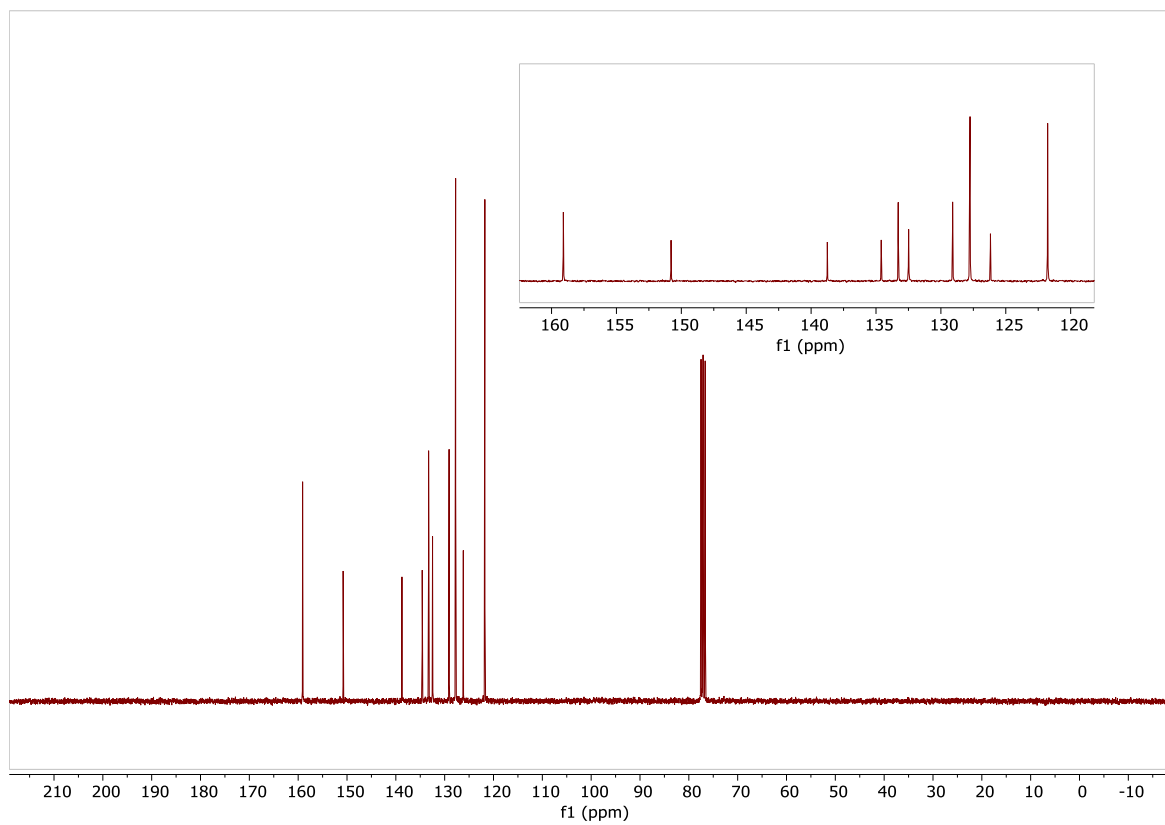


Figure S10. ^{13}C NMR (CDCl_3 , $20\text{ }^\circ\text{C}$) spectrum of $[1,1'-\{4,4'-[(2-\text{BrC}_6\text{H}_4)\text{CH}=\text{N}]_2\text{C}_6\text{H}_4\}]_2$ (**1**).

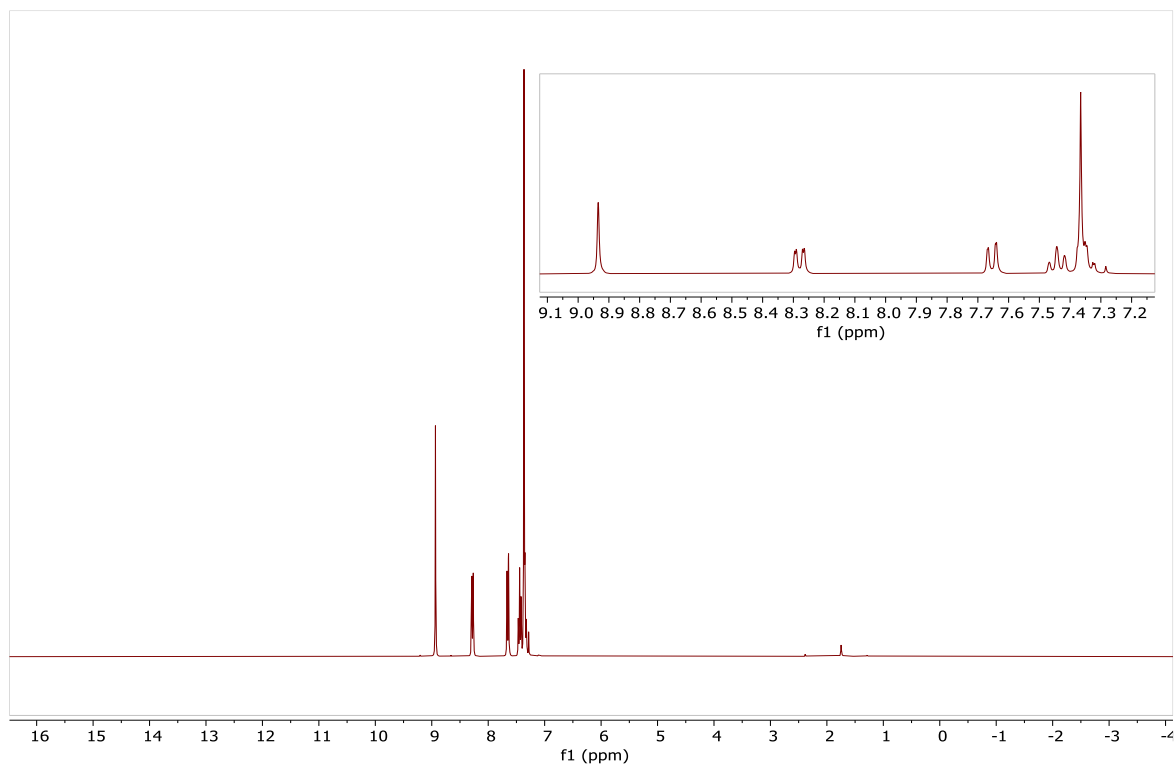


Figure S11. ^1H NMR (CDCl_3 , $20\text{ }^\circ\text{C}$) spectrum of $[1,1'-\{3,3'-(\text{CH}_3)_2-4,4'-[(2-\text{BrC}_6\text{H}_4)\text{CH}=\text{N}]_2\text{C}_6\text{H}_4\}]_2$ (**2**).

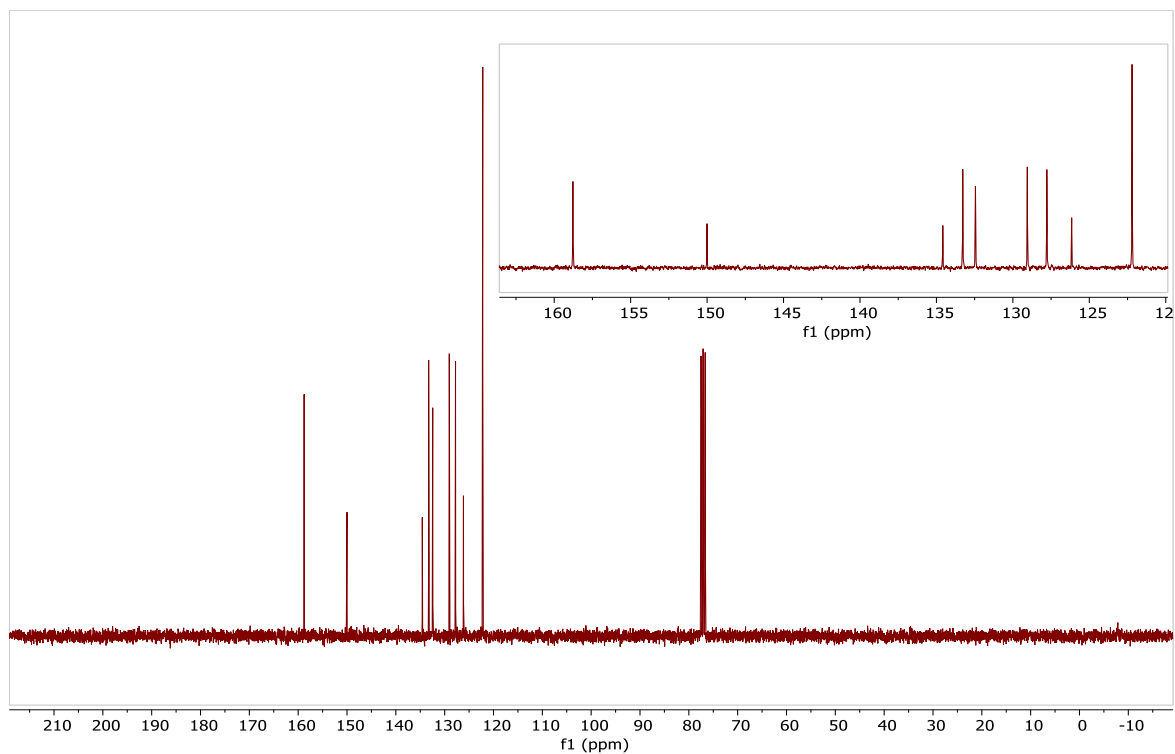


Figure S12. ^{13}C NMR (CDCl_3 , $20\text{ }^\circ\text{C}$) spectrum of $[1,1'\text{-}\{3,3'\text{-(CH}_3)_2\text{-4,4'-}[(2\text{-BrC}_6\text{H}_4)\text{CH=N}]_2\text{C}_6\text{H}_4\}]_2$ (**2**).

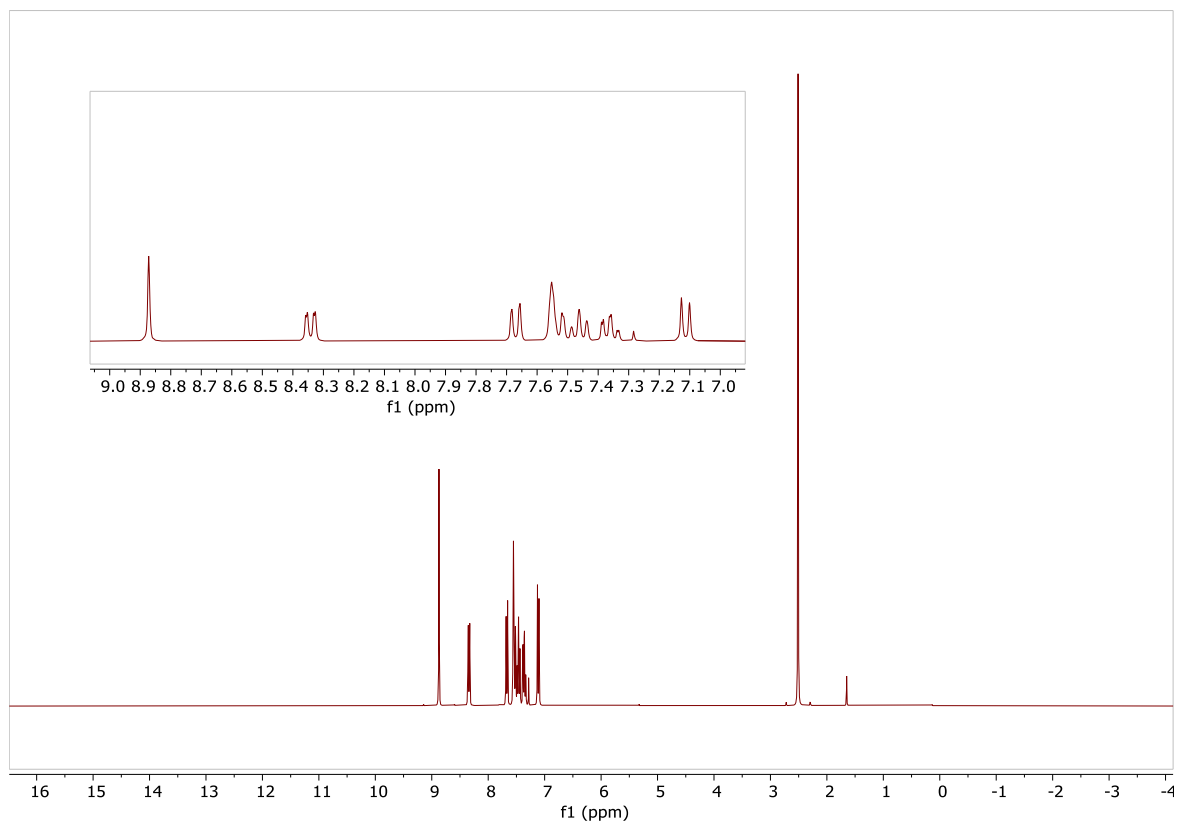


Figure S13. ^1H NMR (CDCl_3 , $20\text{ }^\circ\text{C}$) spectrum of $1,4\text{-}[(2\text{-BrC}_6\text{H}_4)\text{CH=N}]_2\text{C}_6\text{H}_4$ (**3**).

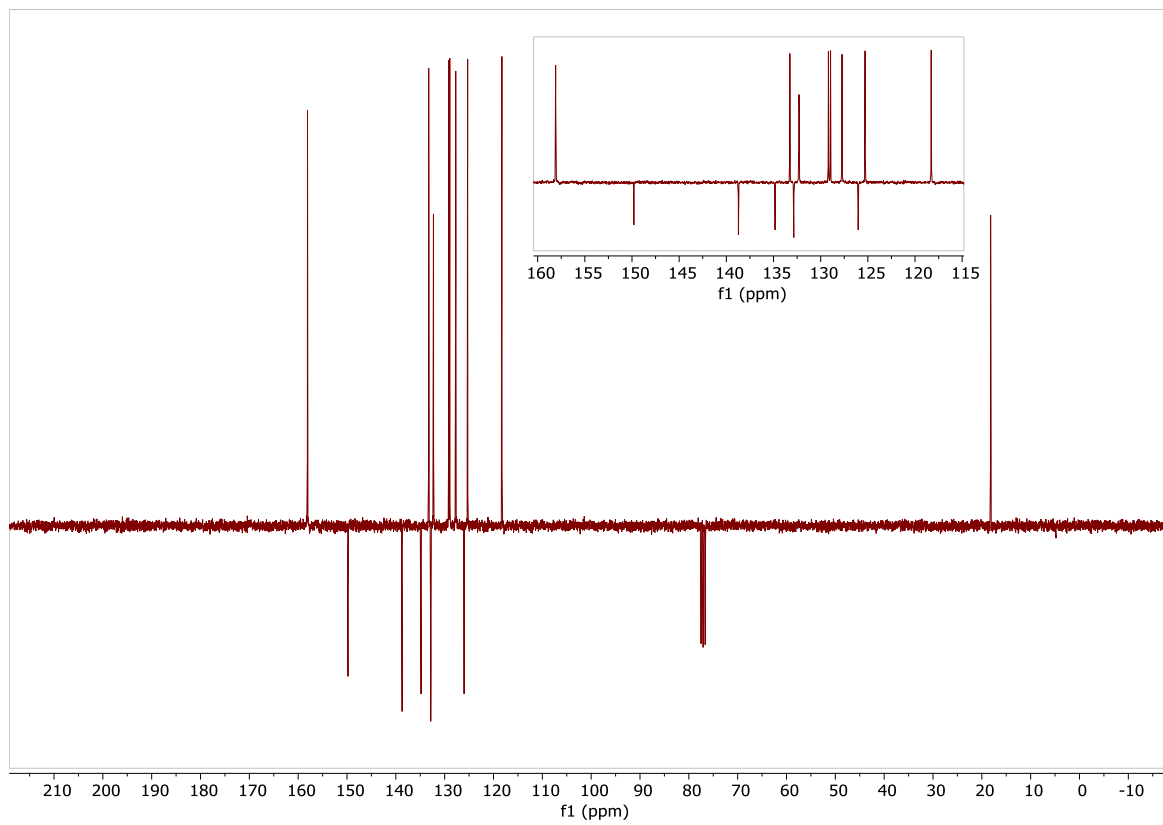


Figure S14. ^{13}C NMR APT (CDCl_3 , 20 °C) spectrum of 1,4-[(2-BrC₆H₄)CH=N]₂C₆H₄ (**3**).

Table S1. Crystal data structure refinement for E,E'-biPh (**1**), E,E'-Me₂biPh (**2**) and E,E'-Ph (**3**)

Compound	1a	1b	1c	2	3
Empirical formula	C ₂₆ H ₁₈ Br ₂ N ₂	C ₂₆ H ₁₈ Br ₂ N ₂	C ₂₆ H ₁₈ Br ₂ N ₂	C ₂₈ H ₂₂ Br ₂ N ₂	C ₂₀ H ₁₄ Br ₂ N ₂
Formula weight	518.24	518.24	518.24	546.30	442.15
Temperature (K)	297(2)	297(2)	297(2)	297(2)	297(2)
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	triclinic	monoclinic	triclinic	triclinic	monoclinic
Space Group	<i>P</i> -1	<i>P</i> 2(1)/ <i>c</i>	<i>P</i> -1	<i>P</i> -1	<i>P</i> 2(1)/ <i>c</i>
Unit cell dimensions					
a (Å)	7.7292(11)	19.680(2)	6.8641(18)	10.1224(13)	14.9043(17)
b (Å)	8.4042(12)	8.2988(9)	9.116(2)	10.5056(14)	6.5540(8)
c (Å)	9.4227(14)	13.8555(16)	17.568(5)	12.5157(16)	8.9163(11)
α (°)	81.672(2)	90	97.476(4)	93.806(2)	90
β (°)	72.598(2)	106.714(2)	94.976(5)	105.503(2)	93.787(2)
γ (°)	65.248(2)	90	94.867(5)	113.368(2)	90
Volume (Å ³)	530.27(13)	1080.7(5)	2167.3(4)	1154.7(3)	869.07(18)
Z	1	4	2	2	2
D _c (mg/cm ³)	1.623	1.588	1.593	1.571	1.690
Absorption coefficient (mm ⁻¹)	3.838	3.756	3.766	3.529	4.667
F(000)	258	1032	516	548	436
Crystal size (mm)	0.31 x 0.26 x 0.14	0.41 x 0.38 x 0.29	0.23 x 0.19 x 0.15	0.34 x 0.28 x 0.13	0.37 x 0.29 x 0.24
θ range for data collection (°)	2.27 to 25.00	2.16 to 25.00	2.26 to 25.00	2.15 to 25.00	1.37 to 25.00
Reflections collected	5147	15194	7643	11136	8046

Independent reflections	1857	3824	3765	4059	1537
	[R(int) = 0.0436]	[R(int) = 0.0514]	[R(int) = 0.0691]	[R(int) = 0.0469]	[R(int) = 0.0420]
Refinement method	Full matrix least-squares on F ²				
Data / restraints / parameters	1857 / 0 / 136	3824 / 0 / 271	3765 / 20 / 271	4059 / 0 / 291	1537 / 0 / 109
Goodness-of-fit on F ²	1.180	1.067	1.179	1.198	1.241
Final R indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0665	<i>R</i> ₁ = 0.0491	<i>R</i> ₁ = 0.1335	<i>R</i> ₁ = 0.0672	<i>R</i> ₁ = 0.0498
	<i>wR</i> ₂ = 0.1264	<i>wR</i> ₂ = 0.1203	<i>wR</i> ₂ = 0.1859	<i>wR</i> ₂ = 0.1213	<i>wR</i> ₂ = 0.1314
R indices (all data)	<i>R</i> ₁ = 0.0905	<i>R</i> ₁ = 0.0794	<i>R</i> ₁ = 0.2314	<i>R</i> ₁ = 0.0824	<i>R</i> ₁ = 0.0644
	<i>wR</i> ₂ = 0.1352	<i>wR</i> ₂ = 0.1300	<i>wR</i> ₂ = 0.2089	<i>wR</i> ₂ = 0.1267	<i>wR</i> ₂ = 0.1515
Largest diff. peak and hole, eÅ ⁻³	0.447 and -0.315	0.767 and -0.414	0.665 and -0.335	0.558 and -0.722	0.425 and -0.427
CCDC	2418174	2418177	2418175	2418176	2418178

