Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences.

Supplementary Material

1,2,4,5-benzenetetracarboxylic acid: A versatile hydrogen bonding template for controlling the regioselective topochemical synthesis of head-to-tail photodimers from stilbazole derivatives.

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Figure S12. ^{1}H NMR spectrum of the photoproduct isolated from the irradiation of (3-Br-Cl-$HStb^+)_2(H_2bta^{2-})$ (**3**): *rctt*-1,3-bis(3-bromophenyl)-2,4-bis(4-pyridyl)cyclobutane.

Figure S13. ^{1}H NMR spectrum of the photoproduct isolated from the irradiation of (4-Br-$HStb^+)_2(H_2bta^{2-})$ (**4**): *rctt*-1,3-bis(4-bromophenyl)-2,4-bis(4-pyridyl)cyclobutane.

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Figure S15. ^{1}H NMR spectrum of the photoproduct isolated from the irradiation of (2-Cl-$HStb^+)_2(H_2bta^{2-})$ (**7** or **8**): *rctt*-1,3-bis(2-chlorophenyl)-2,4-bis(4-pyridyl)cyclobutane.

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Figure S17. From bottom to top: Comparative PXRD patterns simulated and experimental for compound **1** and experimental XRD pattern for compound **9** .

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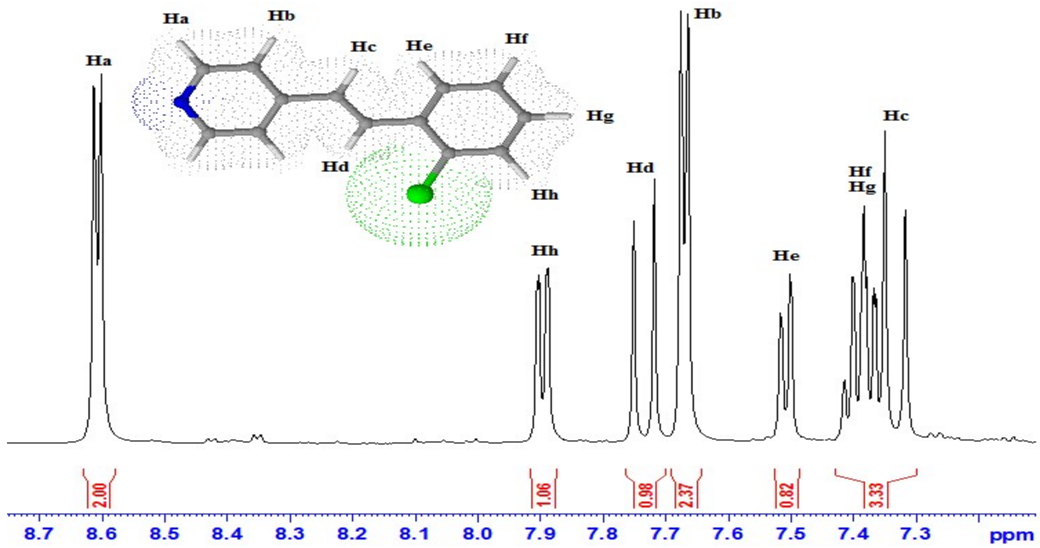
Figure S25. Comparative PXRD patterns simulated (top) and experimental for compound **10** (bottom).

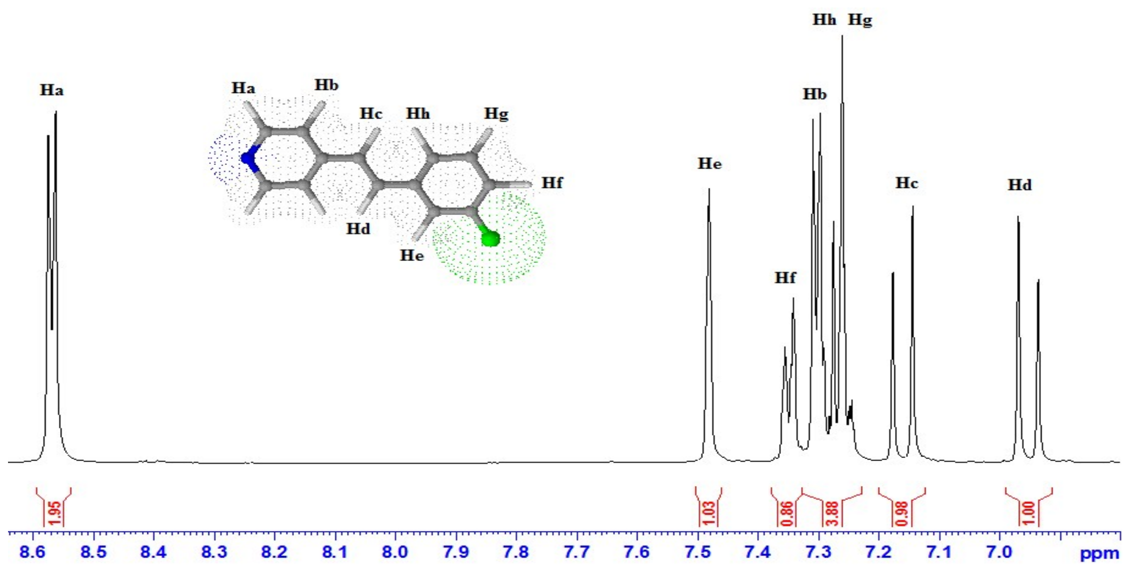
Characterization by ^{1}H NMR **spectroscopy of *Trans*-4-stilbazole Derivatives:**

Figure S1. ^{1}H NMR spectrum of *trans*-2-chlorine-4-stilbazole (2-Cl-Stb).



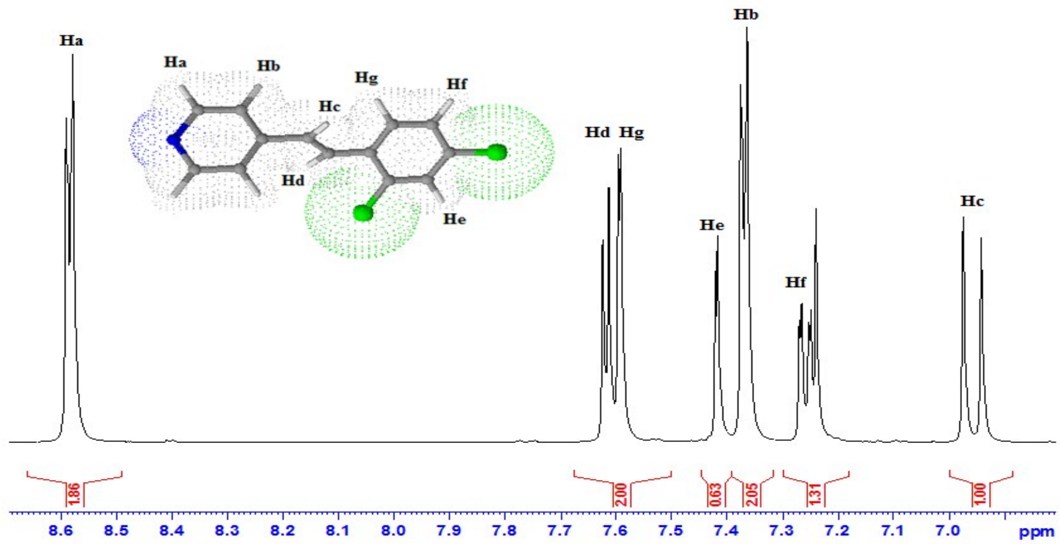
^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.61 (d, 2H, *J*ab = 6.0, Ha), 7.90 (dd, 1H, *J*hg = 8.0, *J*hf = 1.7, Hh), 7.73 (d, 1H, *J*dc = 16.3, Hd), 7.67 (d, 2H, *J*ba = 6.0, Hb), 7.51 (dd, 1H, *J*ef = 8.1, *J*eg = 1.6, He), 7.39 (m, 2H, Hf, Hg), 7.33 (d, 1H, *J*cd = 16.3, Hc) ppm.

Figure S2. ^{1}H NMR spectrum of *trans*-3-chlorine-4-stilbazole (3-Cl-Stb).



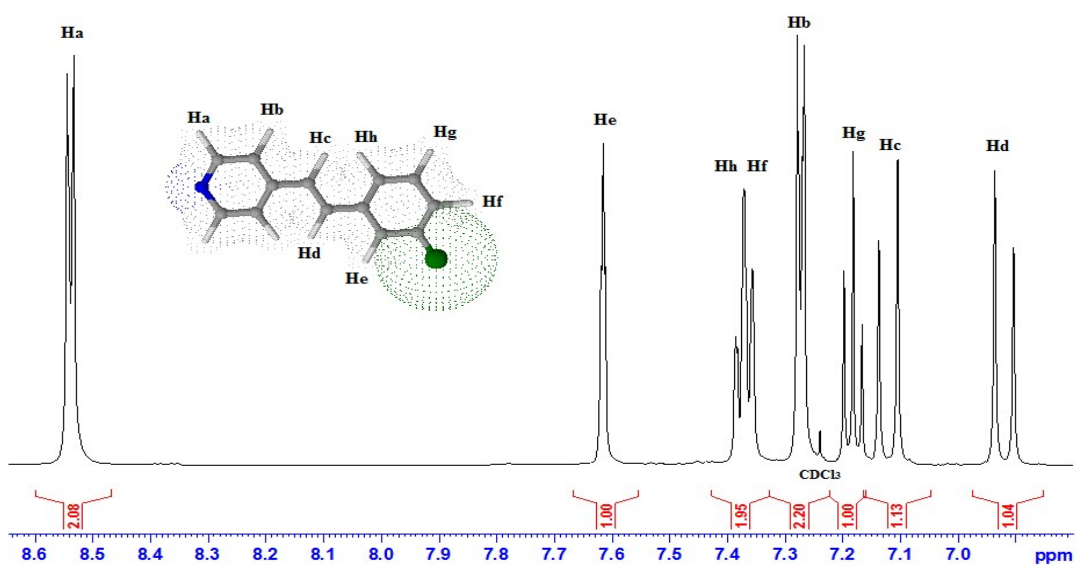
^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.57 (d, 2H, *J*ab = 6.0, Ha), 7.48 (s, 1H, He), 7.35 (dd, 1H, *J*fg = 7.4, Jfh = 1.5, Hf), 7.30 (d, 2H, *J*ba = 6.0, Hb), 7.28 (m, 2H, Hg, Hh), 7.16 (d, 1H, *J*cd = 16.3, Hc), 6.95 (d, 1H, *J*dc = 16.3 Hd) ppm.

Figure S3. ^{1}H NMR spectrum of *trans*-2,4-dichlorine-4-stilbazole (2,4-dCl-Stb).



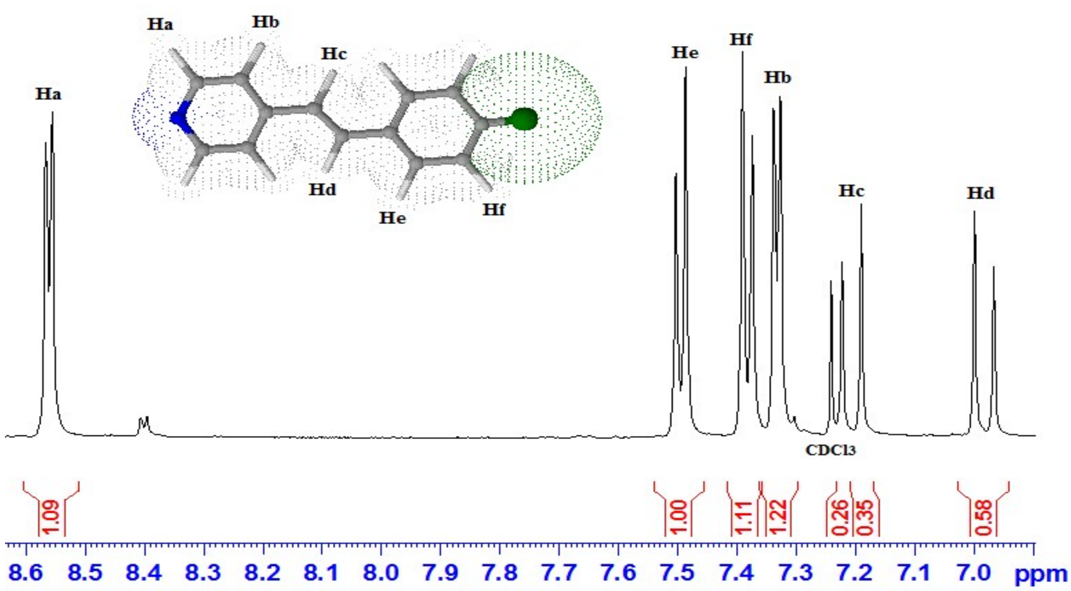
^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.59 (d, 2H, *J*ab = 6.2, Ha), 7.61 (d, 1H, *J*cd = 16.3, Hd), 7.60 (d, 1H, *J*gf = 8.5, Hg), 7.42 (d, 1H, *J*ef = 2.0, He), 7.36 (d, 2H, *J*ba = 6.2, Hb), 7.26 (dd, 1H, *J*fg = 8.5, *J*fe = 2.0, Hf), 6.96 (d, 1H, *J*dc = 16.3, Hc) ppm.

Figure S4. ^{1}H NMR spectrum of *trans*-3-bromine-4-stilbazole (3-Br-Stb).



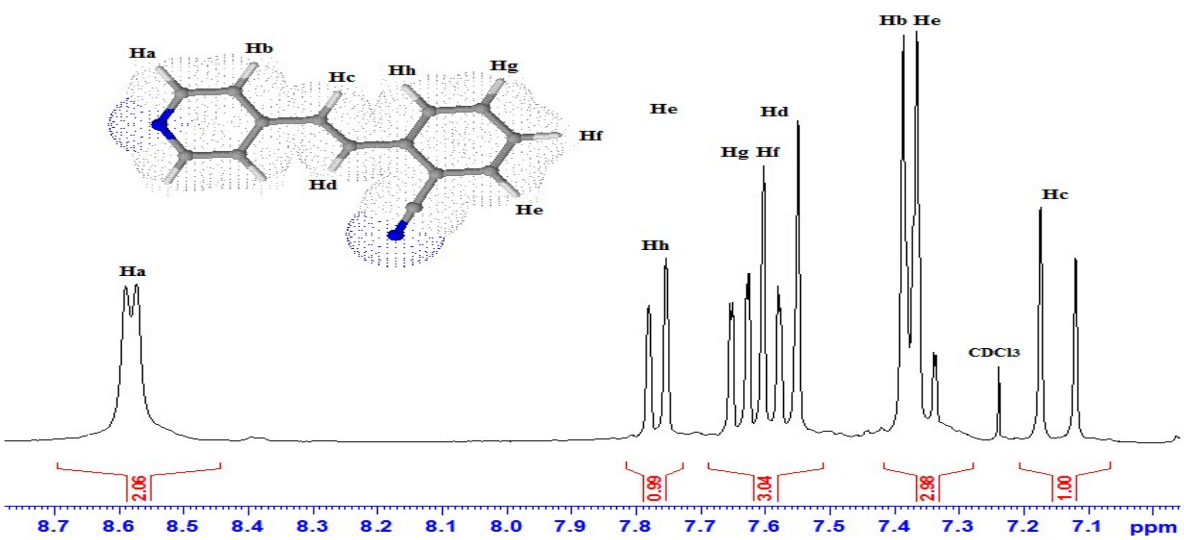
^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.54 (dd, 2H, *J*ab = 5.0, *J*ab′ = 1.3, Ha), 7.62 (m, 1H, He), 7.38 (dd, 1H, *J*hg = 7.6, *J*hf = 2.0, Hh), 7.36 (dd, 1H, *J*fg = 7.2, *J*fh = 2.0, Hf), 7.27 (dd, 2H, *J*ba = 5.0, *J*ba′ = 1.3, Hb), 7.18 (t, 1H, *J*gh = 7.6, *J*gf = 7.2, Hg), 7.12 (d, 1H, *J*cd = 16.3, Hc), 6.92 (d, 1H, *J*dc = 16.3, Hd) ppm.

Figure S5. ^{1}H NMR spectrum of *trans*-4-bromine-4-stilbazole (4-Br-Stb).



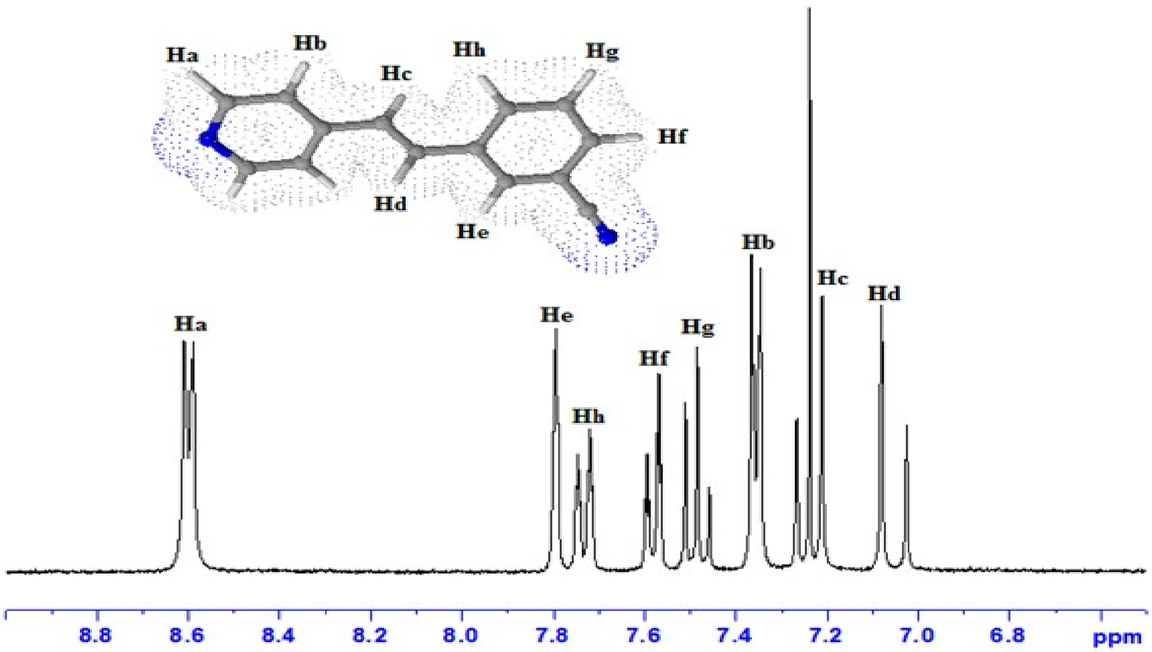
^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.56 (d, 2H, *J*ab = 5.8, Ha), 7.49 (d, 2H, *J*ef = 8.4, He), 7.38 (d, 2H, *J*fe = 8.4, Hf), 7.33 (d, 2H, *J*ba = 5.8, Hb), 7.21 (d, 1H, *J*cd = 16.3, Hc), 6.98 (d, 1H, *J*dc = 16.3, Hd) ppm

Figure S6. ^{1}H NMR spectrum of *trans*-2-benzonitrile-4-stilbazole (2-CN-Stb).



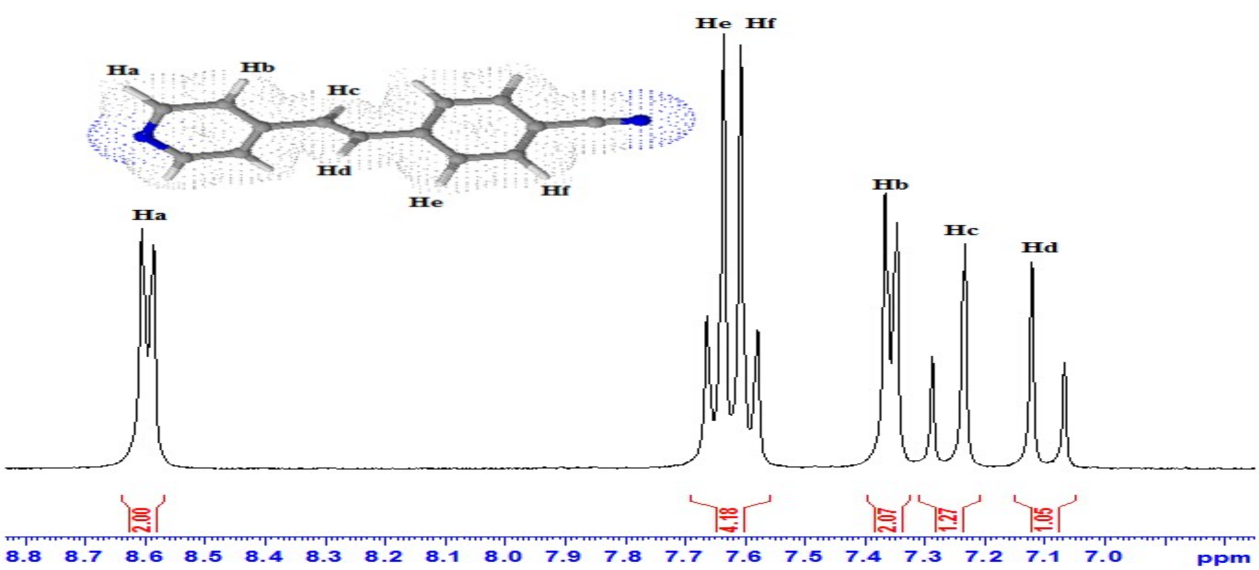
^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.58 (d, 2H, *J*ab = 5.7, Ha), 7.76 (dd, 1H, *J*hg = 7.7, *J*hf = 1.3, Hh), 7.63 (ddd, 1H, *J*gh = 7.7, *J*gf = 7.4, *J*ge = 1.2, Hg), 7.60 (ddd, 1H, *J*fg = *J*fe = 7.4, *J*fh = 1.3, Hf), 7.59 (d, 1H, *J*dc = 16.1, Hd), 7.38 (d, 2H, *J*ba = 5.7, Hb), 7.36 (dd, 1H, *J*ef = 7.4, *J*eg = 1.2, He), 7.14 (d, 1H, *J*cd = 16.1, Hc) ppm.

Figure S7. ^{1}H NMR spectrum of *trans*-3-benzonitrile-4-stilbazole (3-CN-Stb).



^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.60 (d, 2H, *J*ab = 5.3, Ha), 7.80 (s, 1H, He), 7.73 (dd, 1H, *J*hg = 7.8, *J*hf = 1.2, Hh), 7.58 (dd, 1H, *J*fg = 7.8, *J*fh = 1.2, Hf), 7.49 (t, 1H, *J*gf = *J*gh = 7.8, Hg), 7.36 (d, 2H, *J*ba = 5.3, Hb), 7.24 (d, 1H, *J*cd = 16.4, Hc), 7.05 (d, 1H, *J*dc = 16.4, Hd) ppm.

Figure S8. **^{1}H NMR spectrum of *trans*-4-benzonitrile-4-stilbazole (4-CN-Stb).**



^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.60 (d, 2H, *J*ab = 6.0, Ha), 7.65 (d, 2H, *J*ef = 8.4, He), 7.60 (d, 2H, *J*fe = 8.4, Hf), 7.36 (d, 2H, *J*ba = 6.0, Hb), 7.26 (d, 1H, *J*cd = 16.3, Hc), 7.09 (d, 1H, *J*dc = 16.3, Hd) ppm.

Characterization of supramolecular ionic assemblies:

(3-Cl-Hstb$^+$)$_2$(H$_2$bta^{2-}) (1): m.p (°C): 230-232. Anal. Calcd (%) for $C_{36}H_{26}Cl_2N_2O_8$: C, 63.07; H, 3.83; N, 4.09. Found: C, 63.63; H, 3.92; N, 4.48. FT-IR (cm^{-1}, KBr): *ν*(=C-H): 3062, *ν*(N$^+$-H): 2143, ν(C=O): 1690, $\nu_{asim}(CO_2^-)$: 1624, $\nu_{sim}(CO_2^-)$: 1346, *ν*(C-Cl): 1062, *ν*(=C–H): 974.

(2,4-di-Cl-Hstb$^+$)$_2$(H$_2$bta)$^{2-}$ (2): m.p (°C): 224-226. Anal. Calcd (%) for $C_{36}H_{24}Cl_4N_2O_8$: C, 57.31; H, 3.21; N, 3.71. Found: C, 57.76; H, 3.29; N, 4.13. FT-IR (cm^{-1}, KBr): *ν*(=C-H): 3100, *ν*(N$^+$-H): 2162, ν(C=O): 1698, $\nu_{asim}(CO_2^-)$: 1618, $\nu_{sim}(CO_2^-)$: 1340, *ν*(C-Cl): 1051, *ν*(=C–H): 964.

(3-Br-Hstb$^+$)$_2$(H$_2$bta^{2-}) (3): m.p (°C): 226-228. Anal. Calcd (%) for $C_{36}H_{26}Br_2N_2O_8$: C, 55.83; H, 3.39; N, 3.62. Found: C, 56.28; H, 3.49; N, 3.91. FT-IR (cm^{-1}, KBr): *ν*(=C-H): 3099, *ν*(N$^+$-H): 2140, ν(C=O): 1692, $\nu_{asim}(CO_2^-)$: 1622, $\nu_{sim}(CO_2^-)$: 1344, *ν*(-C–Br): 1095, *ν*(=C–H): 976.

(4-Br-Hstb$^+$)$_2$(H$_2$bta^{2-}) (4): m.p (°C): 256-258. Calcd (%) for $C_{36}H_{26}Br_2N_2O_8$: C, 55.83; H, 3.39; N, 3.62. Found: C, 56.54; H, 3.11; N, 4.40. FT-IR (cm^{-1}, KBr): ν(=C-H): 3097, *ν*(N$^+$-H): 2135, ν(C=O): 1688, $\nu_{asim}(CO_2^-)$: 1624, $\nu_{sim}(CO_2^-)$: 1342, *ν*(-C–Br): 1094, ν(=C–H): 972.

(3-CN-Hstb$^+$)$_2$(H$_2$bta^{2-}) (5): m.p (°C): 240-242. Anal. Calcd (%) for $C_{38}H_{26}N_4O_8$: C, 68.46; H, 3.94; N, 8.40. Found: C, 67.46; H, 4.32; N, 8.14. FT-IR (cm^{-1}, KBr): *ν*(=C-H): 3065, *ν*(–CN): 2229, *ν*(N$^+$-H): 2148, *ν*(C=O): 1688, $\nu_{asim}(CO_2^-)$: 1624, $\nu_{sim}(CO_2^-)$: 1343, ν(=C–H): 982.

(2-CN-Hstb$^+$)$_2$(H$_2$bta^{2-}) (6): m.p (°C): 223-225. Anal. Calcd (%) for $C_{38}H_{26}N_4O_8$: C, 68.46; H, 3.94; N, 8.40. Found: C, 69.08; H, 3.82; N, 9.02. FT-IR (cm^{-1}, KBr): *ν*(=C-H): 3065, *ν*(–CN): 2227, *ν*(N$^+$-H): 2130, *ν*(C=O): 1704, $\nu_{asim}(CO_2^-)$: 1628, $\nu_{sim}(CO_2^-)$: 1456, *ν*(=C–H): 985.

(2-Cl-Hstb$^+$)$_2$(H$_2$bta^{2-}) (7): m.p (°C): 203-205. Anal. Calcd (%) for $C_{36}H_{26}Cl_2N_2O_8$: C, 63.07; H, 3.83; N, 4.09. Found: C, 63.01; H, 3.88; N, 4.18. FT-IR (cm^{-1}, KBr): *ν*(=C-H): 3066, *ν*(N$^+$-H): 2148, ν(C=O): 1718, $\nu_{asim}(CO_2^-)$: 1624, $\nu_{sim}(CO_2^-)$: 1336, *ν*(C-Cl): 1049, *ν*(=C–H): 974.

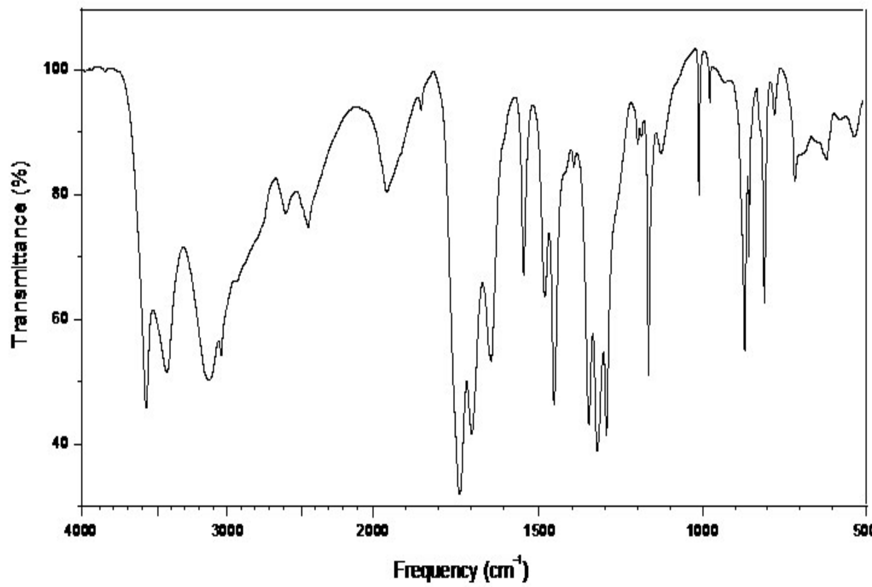
(2-Cl-Hstb$^+$)$_2$(H$_2$bta^{2-}) (8): m.p (°C): 208-210. Anal. Calcd (%) for $C_{36}H_{26}Cl_2N_2O_8$: C, 63.07; H, 3.83; N, 4.09. Found: C, 63.19; H, 3.86; N, 4.48. FT-IR (cm^{-1}, KBr): *ν*(=C-H): 3095, *ν*(N$^+$-H): 2160, ν(C=O): 1695, $\nu_{asim}(CO_2^-)$: 1618, $\nu_{sim}(CO_2^-)$: 1344, *ν*(C-Cl): 1047, *ν*(=C–H): 975.

(3-Cl-Hstb$^+$)$_2$(H$_2$bta^{2-}) (9): m.p (°C): 234-236. Anal. Calcd (%) for $C_{36}H_{26}Cl_2N_2O_8$: C, 63.07; H, 3.83; N, 4.09. Found: C, 63.00; H, 3.87; N, 4.05. FT-IR (cm^{-1}, KBr): *ν*(=C-H): 3063, *ν*(N$^+$-H): 2145, ν(C=O): 1687, $\nu_{asim}(CO_2^-)$: 1626, $\nu_{sim}(CO_2^-)$: 1346, *ν*(C-Cl): 1063, *ν*(=C–H): 978.

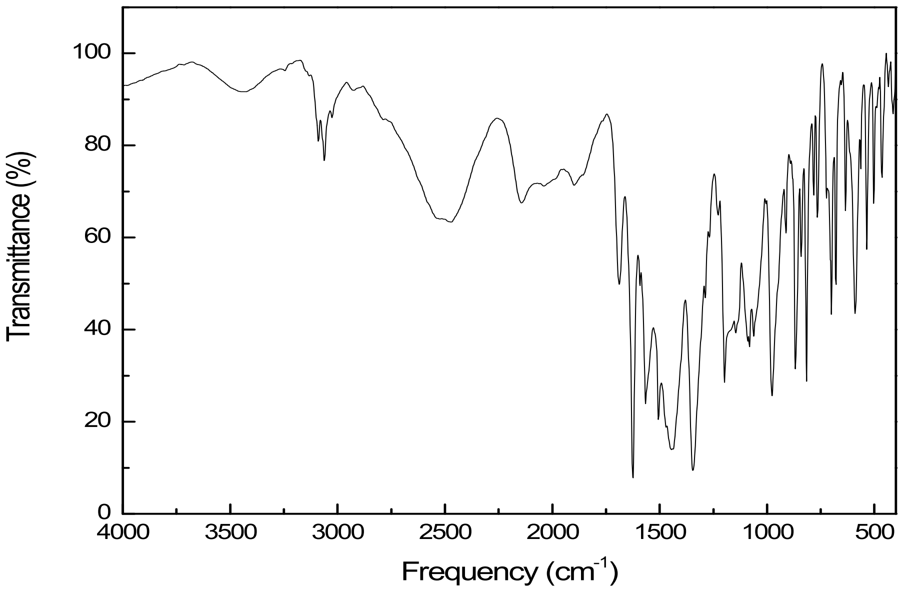
$(4\text{-CN-Hstb}^+)_2(H_2bta^{2-})$ (10): m.p (°C): 248-250. Anal. Calcd (%) for $C_{38}H_{26}N_4O_8$: C, 68.46; H, 3.94; N, 8.40. Found: C, 67.64; H, 4.42; N, 8.05. FT-IR (cm^{-1}, KBr): ν(=C-H): 3065, ν(−CN): 2228, $\nu(N^+\text{-}H)$: 2151, ν(C=O): 1703, $\nu_{asim}(CO_2^-)$: 1626, $\nu_{sim}(CO_2^-)$: 1452, ν(=C–H): 985.

Figure S9. FT-IR spectra of 1,2,4,5-benzenetetracarboxylic acid (H_4bta) (a) and compounds **1-10** in KBr disk (b-k).

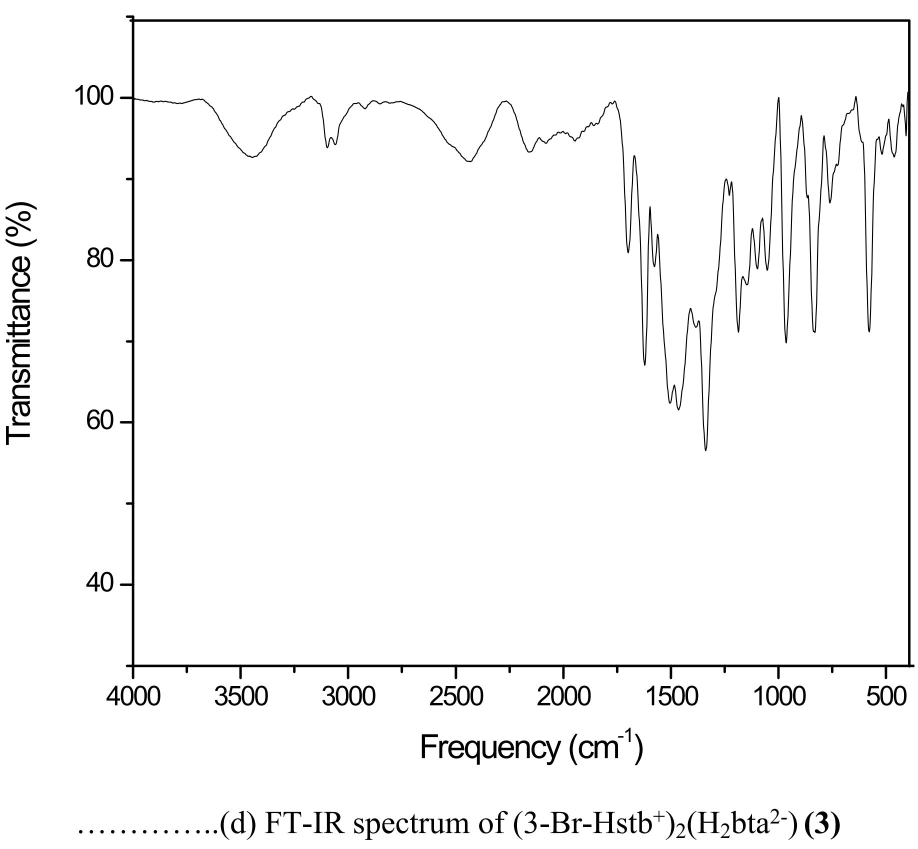
(a) FT-IR spectrum of 1,2,4,5-benzenetetracarboxylic acid (H_4bta)



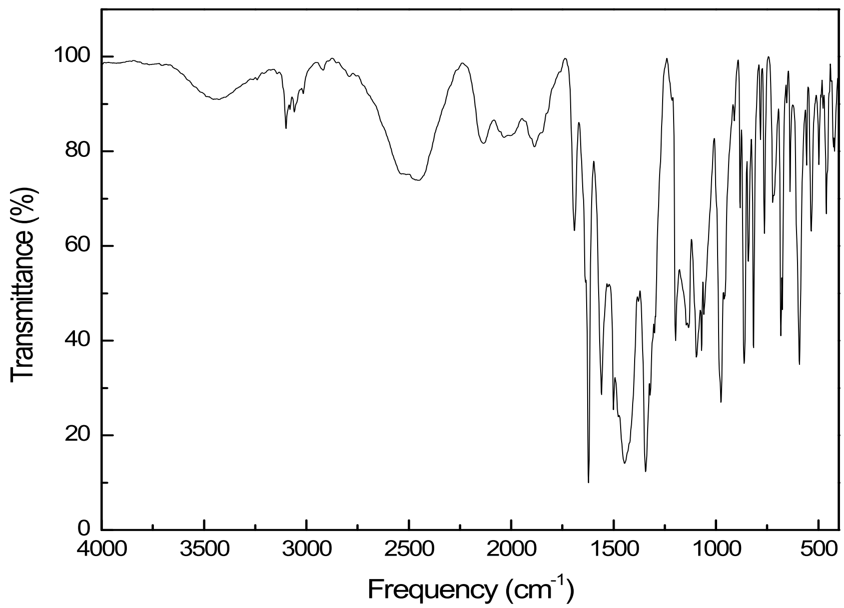
(b) FT-IR spectrum of $(3\text{-Cl-Hstb}^+)_2(H_2bta^{2-})$ **(1)**



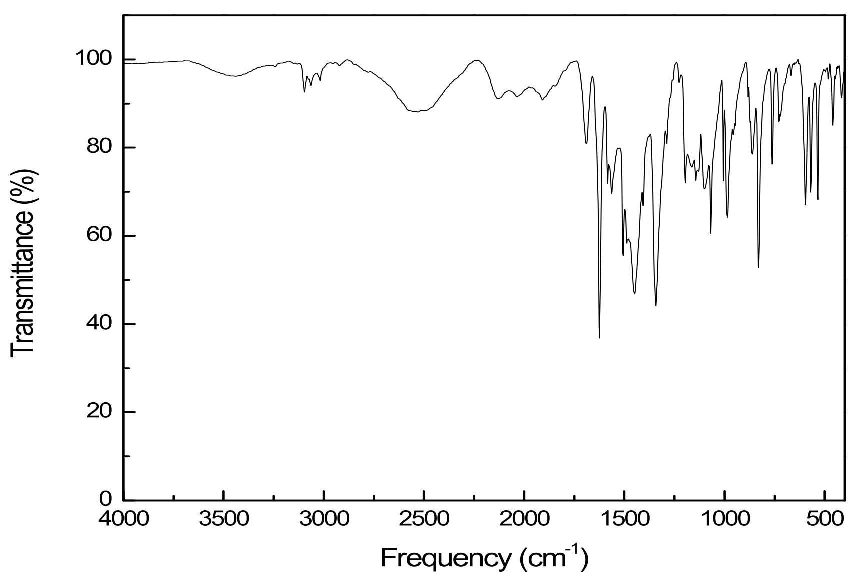
(c) FT-IR spectrum of (2,4-di-Cl-Hstb$^+$)$_2$(H$_2$bta)$^{2-}$ **(2)**



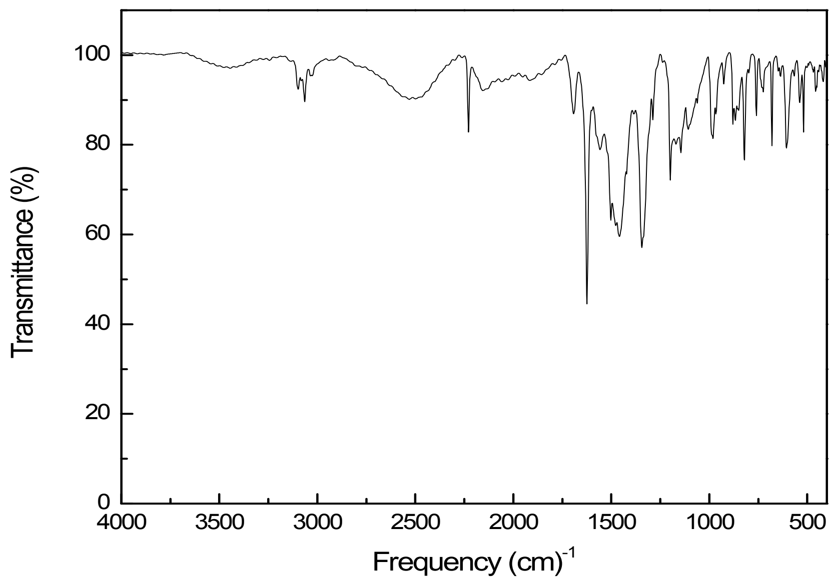
…………..(d) FT-IR spectrum of (3-Br-Hstb$^+$)$_2$(H$_2$bta^{2-}) **(3)**



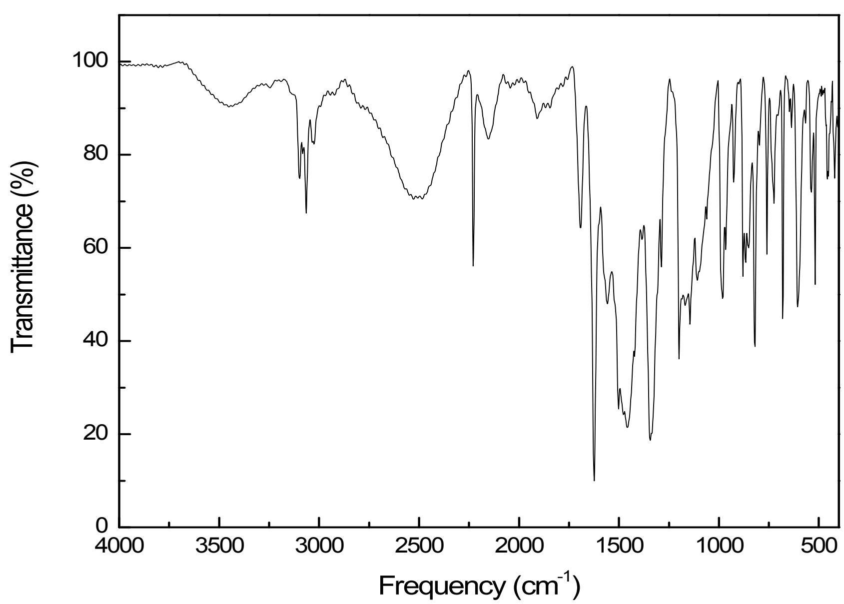
(e) FT-IR spectrum of $(4\text{-Br-Hstb}^{+})_2(H_2bta^{2-})$ **(4)**



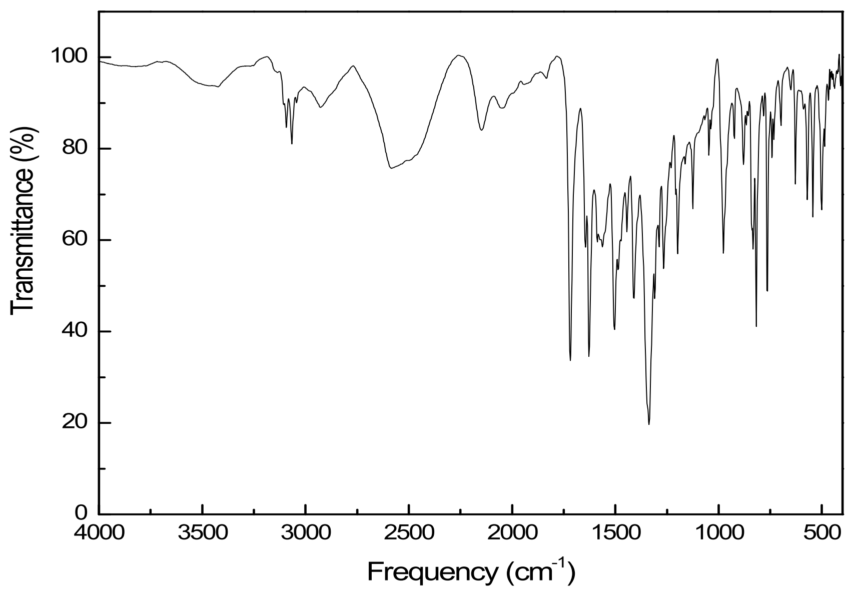
(f) FT-IR spectrum of $(3\text{-CN-Hstb}^{+})_2(H_2bta^{2-})$ **(5)**



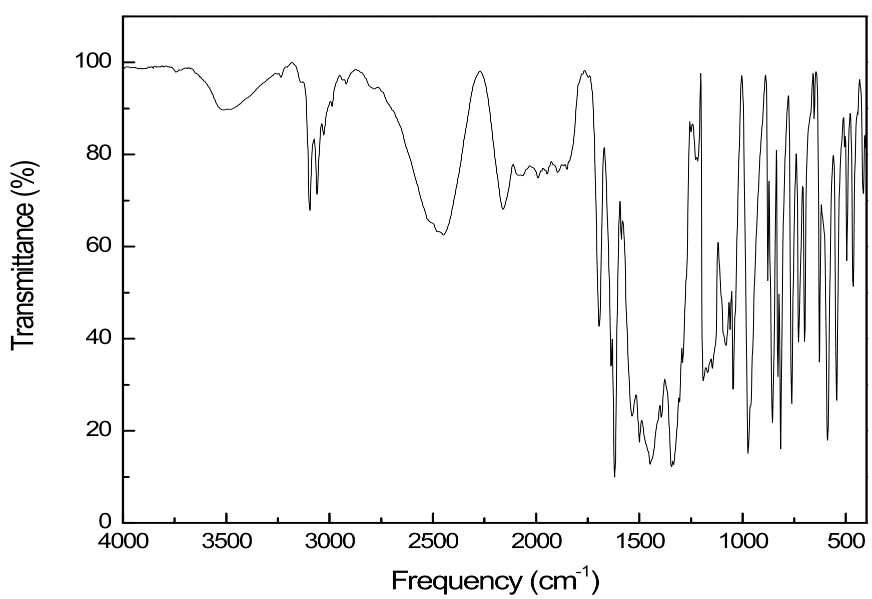
(g) FT-IR spectrum of $(2\text{-CN-Hstb}^{+})_2(H_2bta^{2-})$ **(6)**



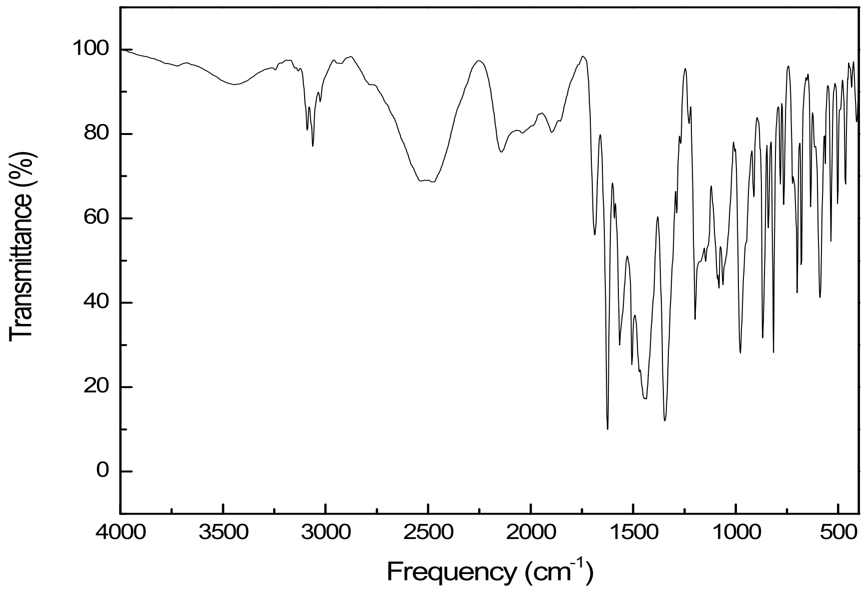
(h) FT-IR spectrum of $(2\text{-Cl-Hstb}^{+})_2(H_2bta^{2-})$ **(7)**



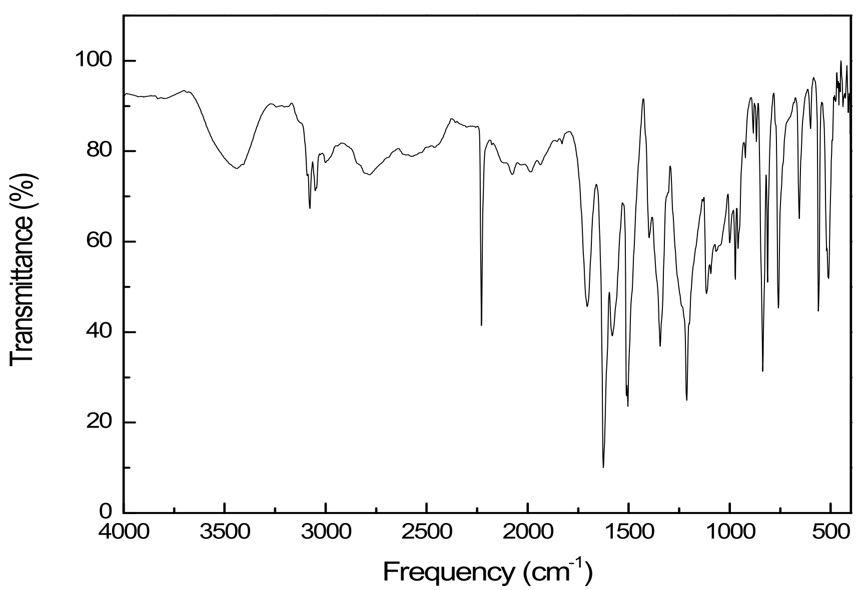
(i) FT-IR spectrum of $(2\text{-Cl-Hstb}^{+})_2(H_2bta^{2-})$ **(8)**



(j) FT-IR spectrum of $(3\text{-Cl-Hstb}^{+})_2(H_2bta^{2-})$ **(9)**

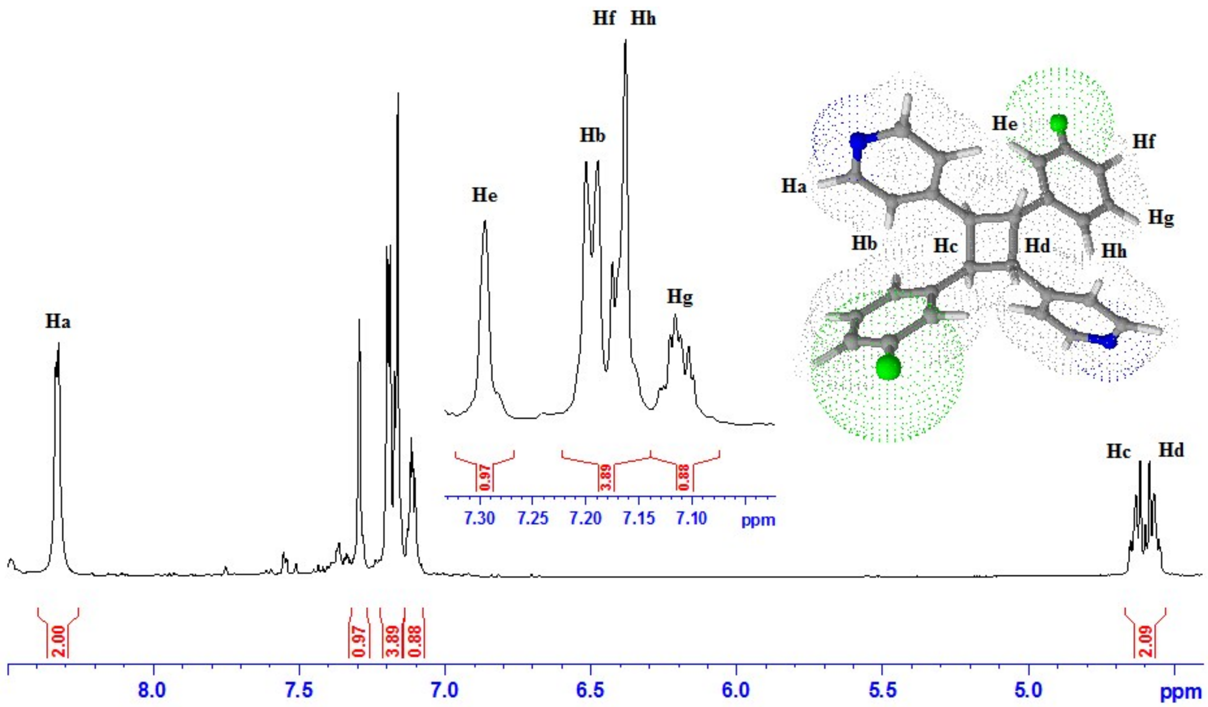


(k) FT-IR spectrum of $(4\text{-CN-Hstb}^{+})_2(H_2bta^{2-})$ **(10)**



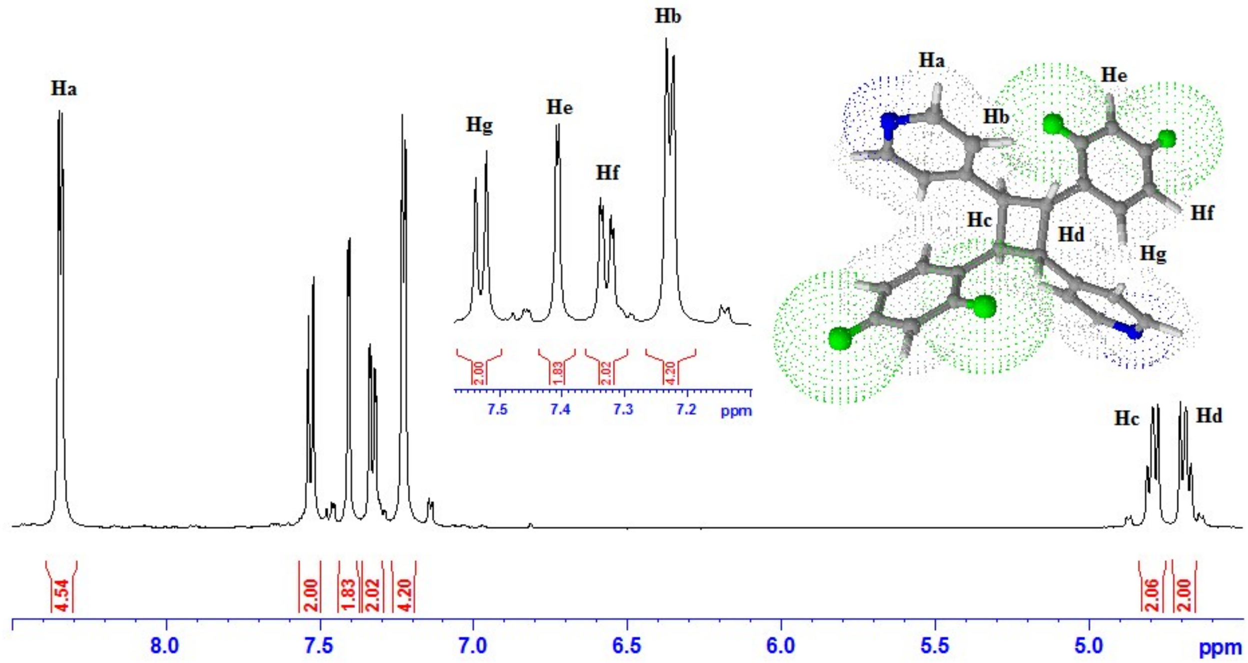
Solid-State Reactivity:

Figure S10. ^{1}H NMR spectrum of the photoproduct isolated from the irradiation of (3-Cl-$HStb^{+})_2(H_2bta^{2-})$ (**1** or **9**): *rctt*-1,3-bis(3-chlorophenyl)-2,4-bis(4-pyridyl)cyclobutane.



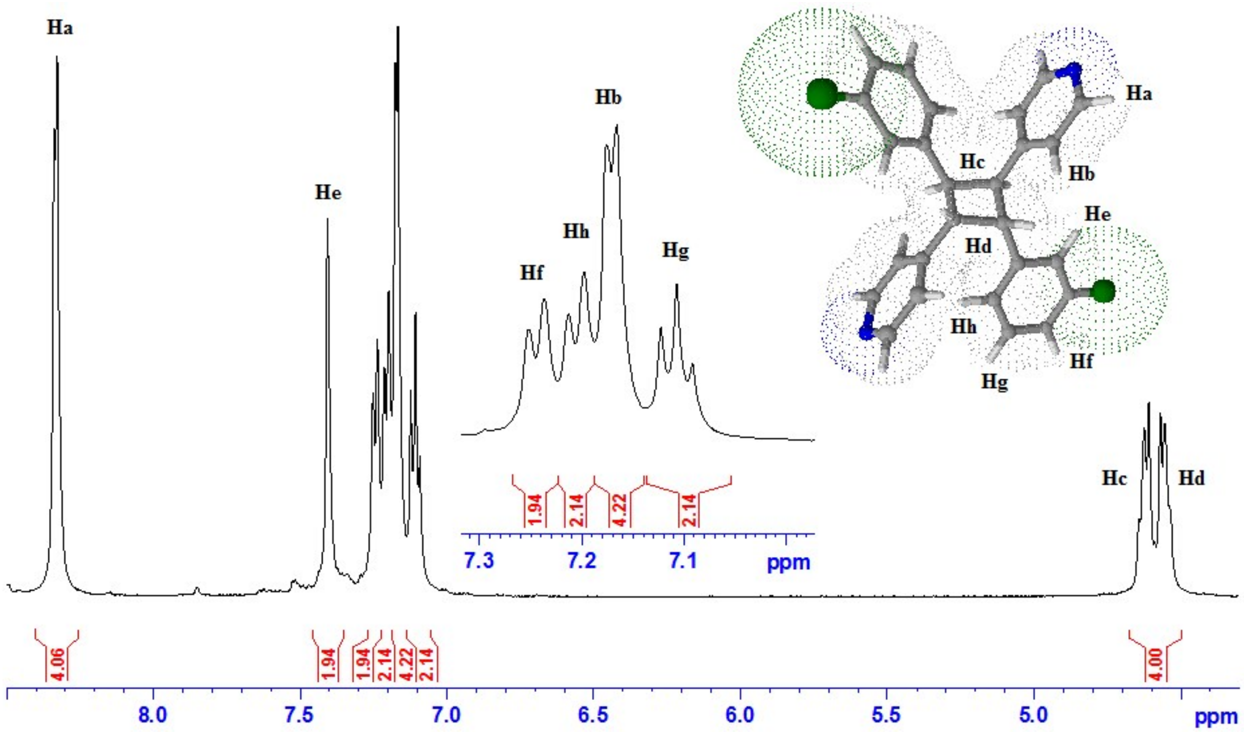
Yield: 86-90%. ^{1}H NMR (DMSO-d_6, 500 MHz) δ 8.33 (d, 4H, *J*ab = 5.0, Ha), 7.29 (s, 2H, He), 7.19 (d, 4H, *J*ba = 5.0, Hb), 7.17 (m, 4H, Hf, Hh), 7.12 (m, 2H, Hg), 4.64 (m, 2H, Hc), 4.56 (m, 2H, Hd) ppm.

Figure S11. ^{1}H NMR spectrum of the photoproduct isolated from the irradiation of (2,4-di-Cl-HStb$^+$)$_2$(H$_2$bta^{2-}) (**2**): *rctt*-1,3-bis(2,4-dichlorophenyl)-2,4-bis(4-pyridyl)cyclobutane.



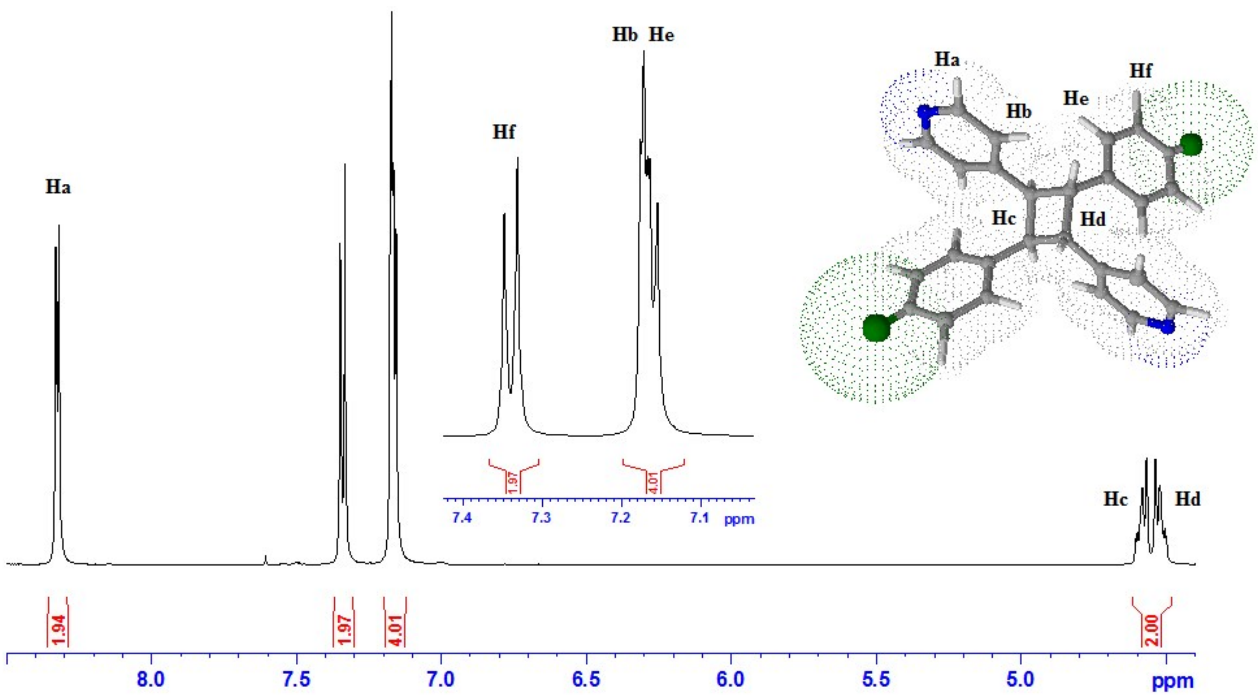
Yield: 91 %. [1]H NMR (DMSO-d_6, 500 MHz) δ 8.34 (d, 4H, *J*ab = 5.8, Ha), 7.53 (d, 2H, *J*gf = 8.4, Hg), 7.41 (d, 2H, *J*ef = 2.0, He), 7.33 (dd, 2H, *J*fg = 8.4, *J*fe = 2.0, Hf), 7.23 (d, 4H, *J*ba = 5.8, Hb), 4.80 (m, 2H, Hc), 4.70 (m, 2H, Hd) ppm.

Figure S12. ^{1}H NMR spectrum of the photoproduct isolated from the irradiation of (3-Br-Cl-HStb$^+$)$_2$(H_2bta^{2-}) (**3**): *rctt*-1,3-bis(3-bromophenyl)-2,4-bis(4-pyridyl)cyclobutane.



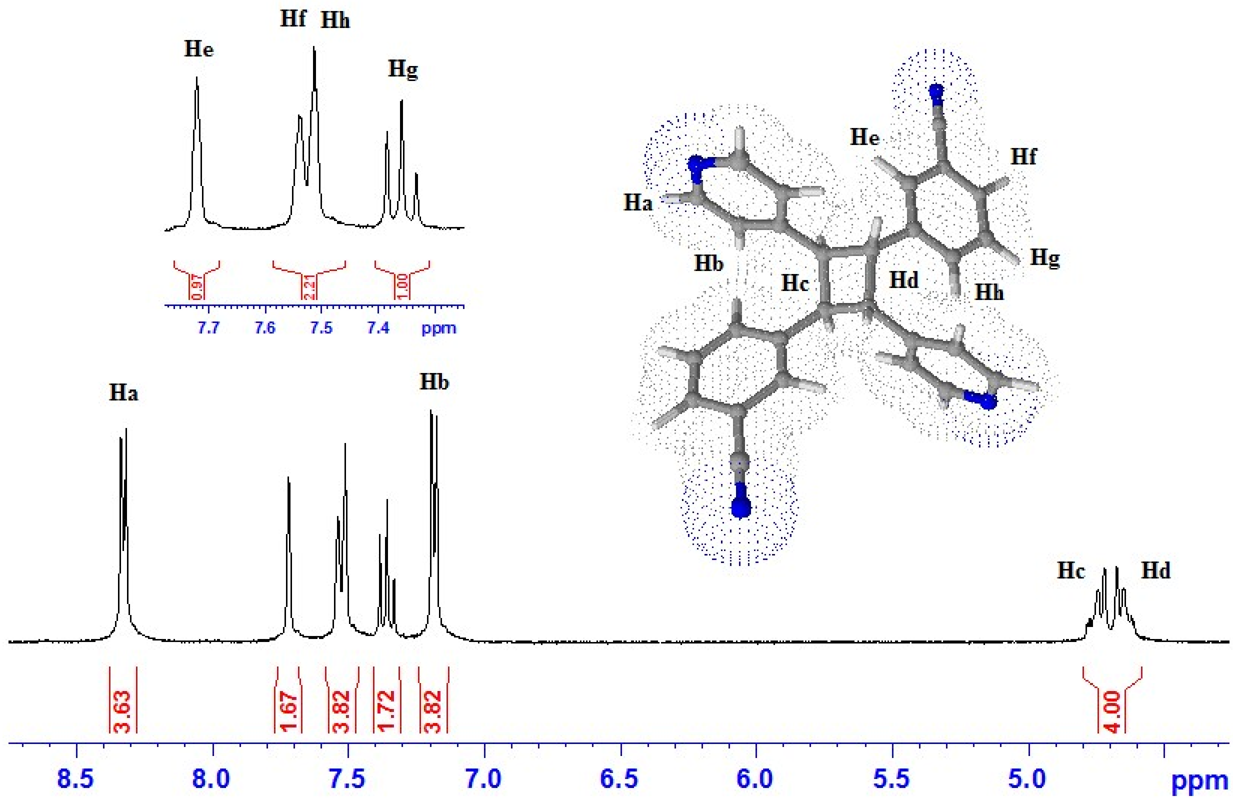
Yield: 86 %. ^{1}H NMR (DMSO-d_6, 500 MHz) δ 8.33 (d, 4H, *J*ab = 4.8, Ha), 7.41 (s, 2H, He), 7.24 (d, 2H, *J*fg = 7.7, Hf), 7.20 (d, 2H, *J*hg = 7.7, Hh), 7.17 (d, 4H, *J*ba = 4.8, Hb), 7.11 (t, 2H, *J*gh = *J*gf = 7.7, Hg), 4.63 (m, 2H, Hc), 4.55 (m, 2H, Hd) ppm.

Figure S13. ^{1}H NMR spectrum of the photoproduct isolated from the irradiation of (4-Br-HStb$^+$)$_2$(H$_2$bta^{2-}) (**4**): *rctt*-1,3-bis(4-bromophenyl)-2,4-bis(4-pyridyl)cyclobutane.



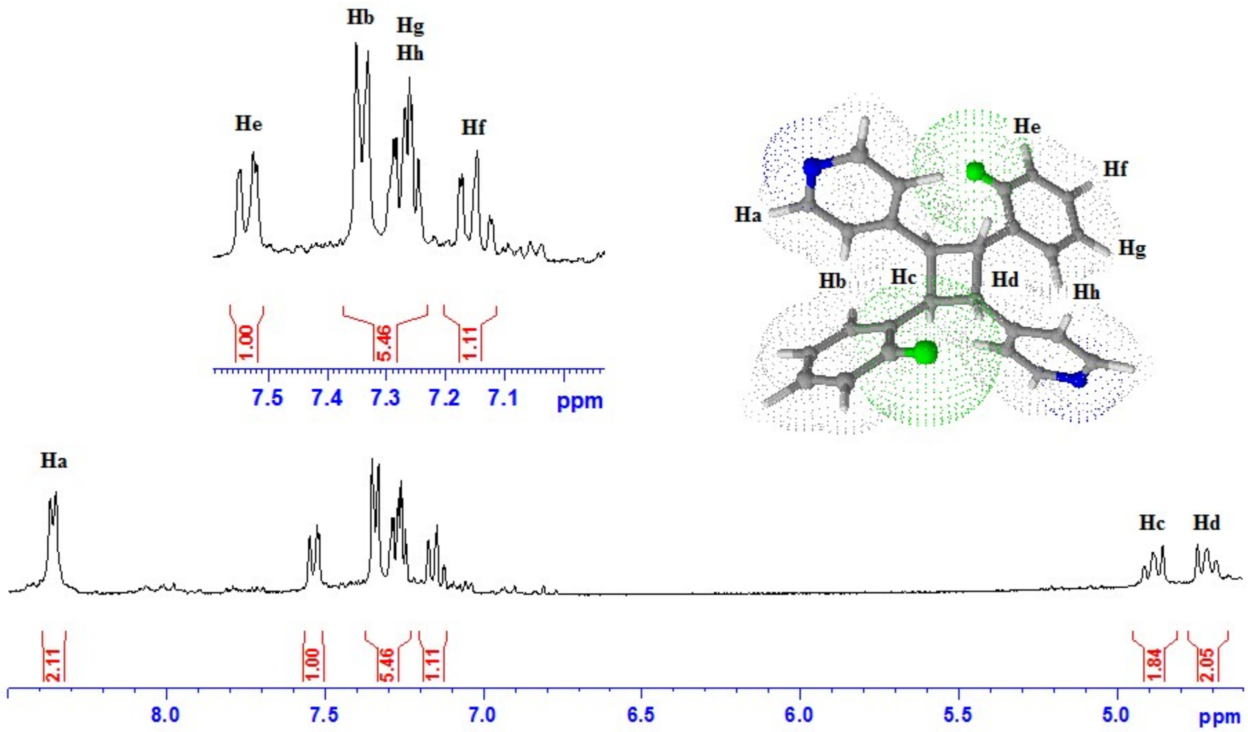
Yield: 98%. ^{1}H NMR (DMSO-d_6, 500 MHz) δ 8.32 (d, 4H, *J*ab = 5.6, Ha), 7.34 (d, 4H, *J*fe = 8.2, Hf), 7.17 (m, 8H, Hb, He), 4.57 (m, 2H, Hc), 4.53 (m, 2H, Hd) ppm.

Figure S14. ^{1}H NMR spectrum of the photoproduct isolated from the irradiation of (3-CN-HStb$^+$)$_2$ (H$_2$bta^{2-}) (**5**): *rctt*-1,3-bis(3-benzonitrile)-2,4-bis(4-pyridyl)cyclobutane.



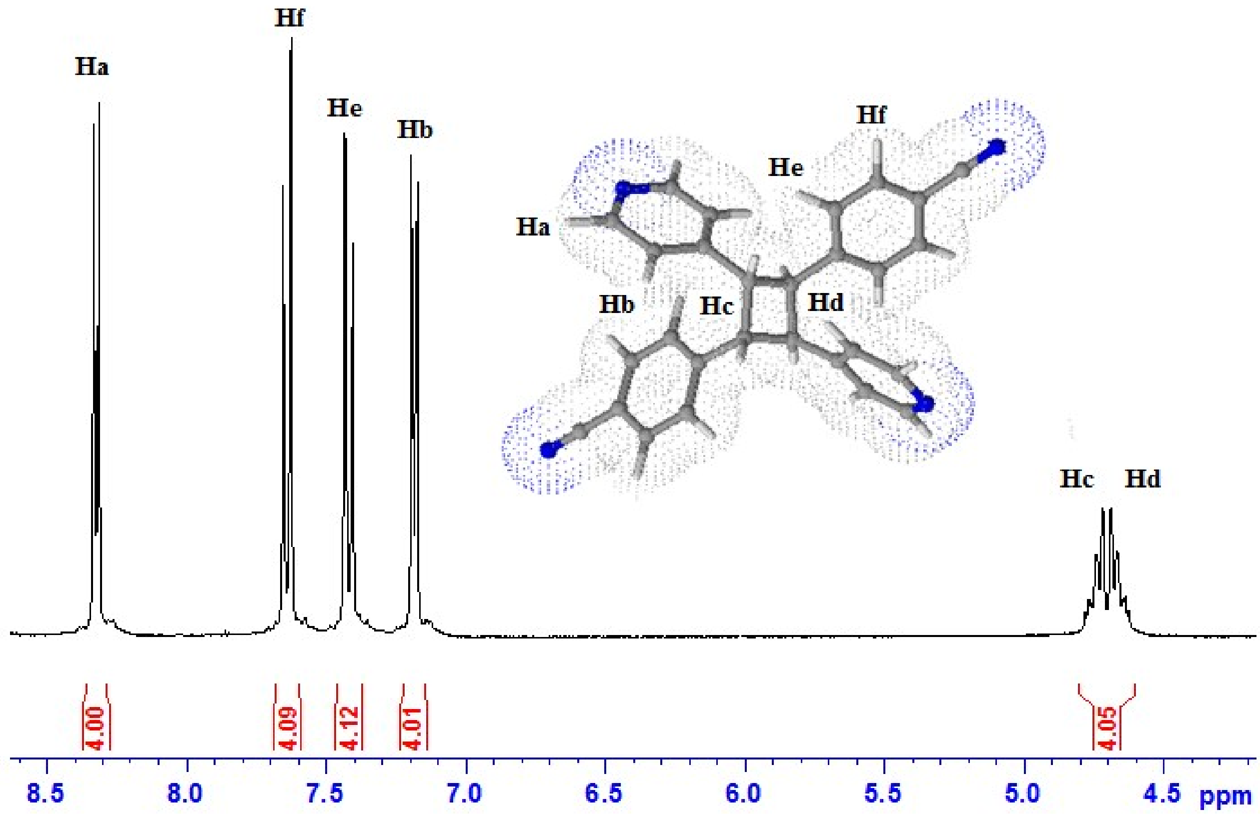
Yield: 100.00 %. ^{1}H NMR (DMSO-$d_{6,}$ 300 MHz) δ 8.33 (d, 4H, *J*ab = 5.3, Ha), 7.72 (s, 2H, He), 7.52 (m, 4H, Hf, Hh), 7.36 (t, 2H, *J*gf = *J*gh = 8.1, Hg), 7.19 (dd, 4H, *J*ba = 5.3, *J*bb′ = 1.4, Hb), 4.76 (m, 2H, Hc), 4.64 (m, 2H, Hd) ppm.

Figure S15. ^{1}H NMR spectrum of the photoproduct isolated from the irradiation of (2-Cl-HStb^{+})$_2$(H$_2$bta^{2-}) (**7** or **8**): *rctt*-1,3-bis(2-chlorophenyl)-2,4-bis(4-pyridyl)cyclobutane.



Yield: 83-85%. ^{1}H NMR (DMSO-$d_{6,}$ 300 MHz) δ 8.36 (d, 4H, *J*ab = 5.8, Ha), 7.53 (dd, 2H, *J*ef = 8.0, *J*eg = 2.0, He), 7.34 (d, 4H, *J*ba = 5.8, Hb), 7.27 (m, 4H, Hg, Hh), 7.16 (ddd, 2H, *J*fg = *J*fe = 8.0, *J*fh = 1.8, Hf), 4.89 (m, 2H, Hc), 4.71 (m, 2H, Hd) ppm.

Figure S16. ^{1}H NMR spectrum of the photoproduct isolated from the irradiation of (4-CN-HStb^{+})$_2$ (H$_2$bta^{2-}) (**10**): *rctt*-1,3-bis(4-benzonitrile)-2,4-bis(4-pyridyl)cyclobutane.



Yield: 100.00 %. ^{1}H NMR (DMSO-$d_{6,}$ 300 MHz) δ 8.32 (dd, 4H, *J*ab = 4.5; *J*ab´= 1.5, Ha), 7.64 (d, 4H, *J*fe = 8.4, Hf), 7.42 (d, 4H, *J*ef = 8.4, He), 7.18 (dd, 4H, *J*ba = 4.5; *J*ba´= 1.5, Hb), 4.73 (m, 2H, Hc), 4.68 (m, 2H, Hd) ppm.

Figure S17. From bottom to top: Comparative PXRD patterns simulated and experimental for compound **1** and experimental XRD pattern for compound **9** (top).

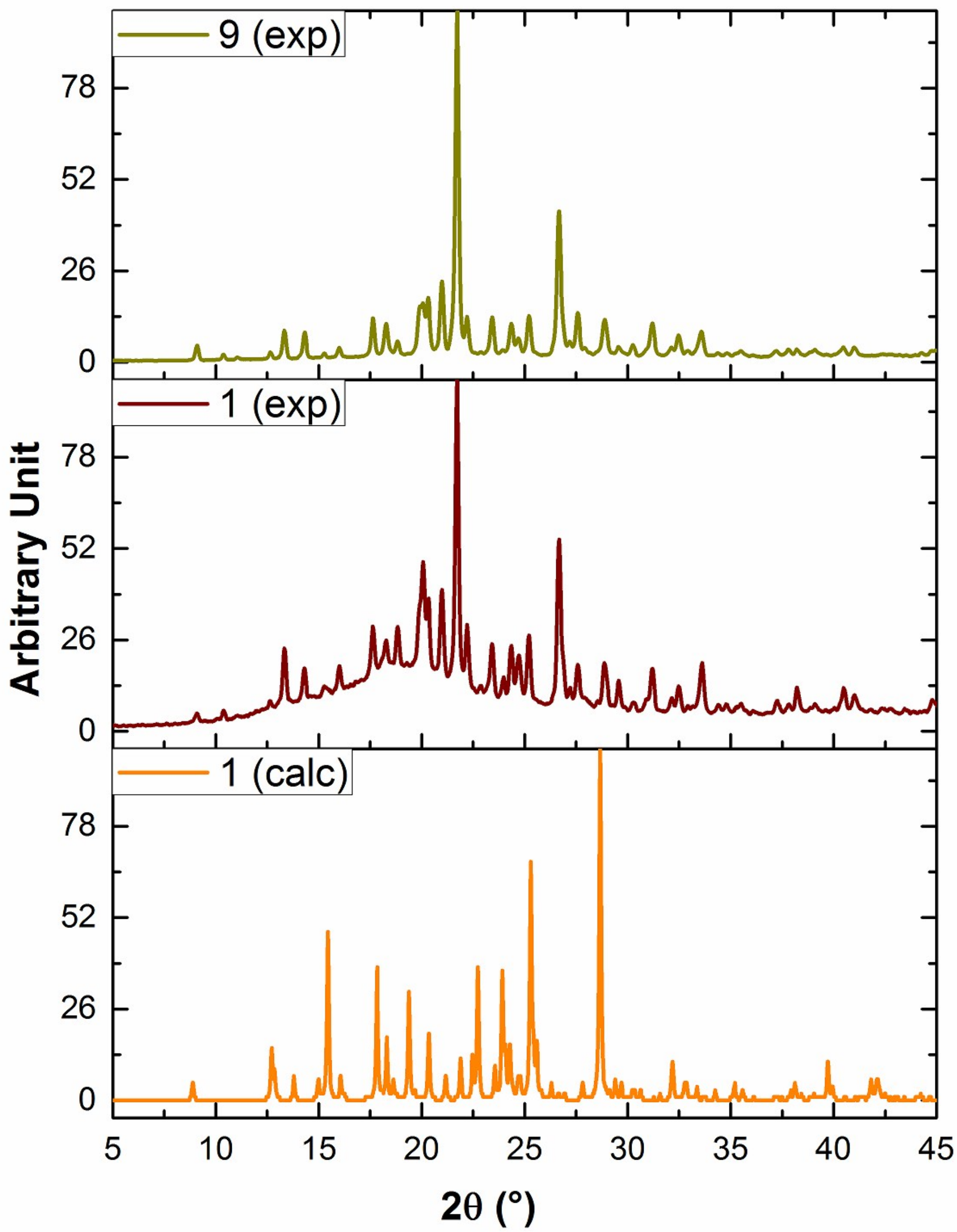
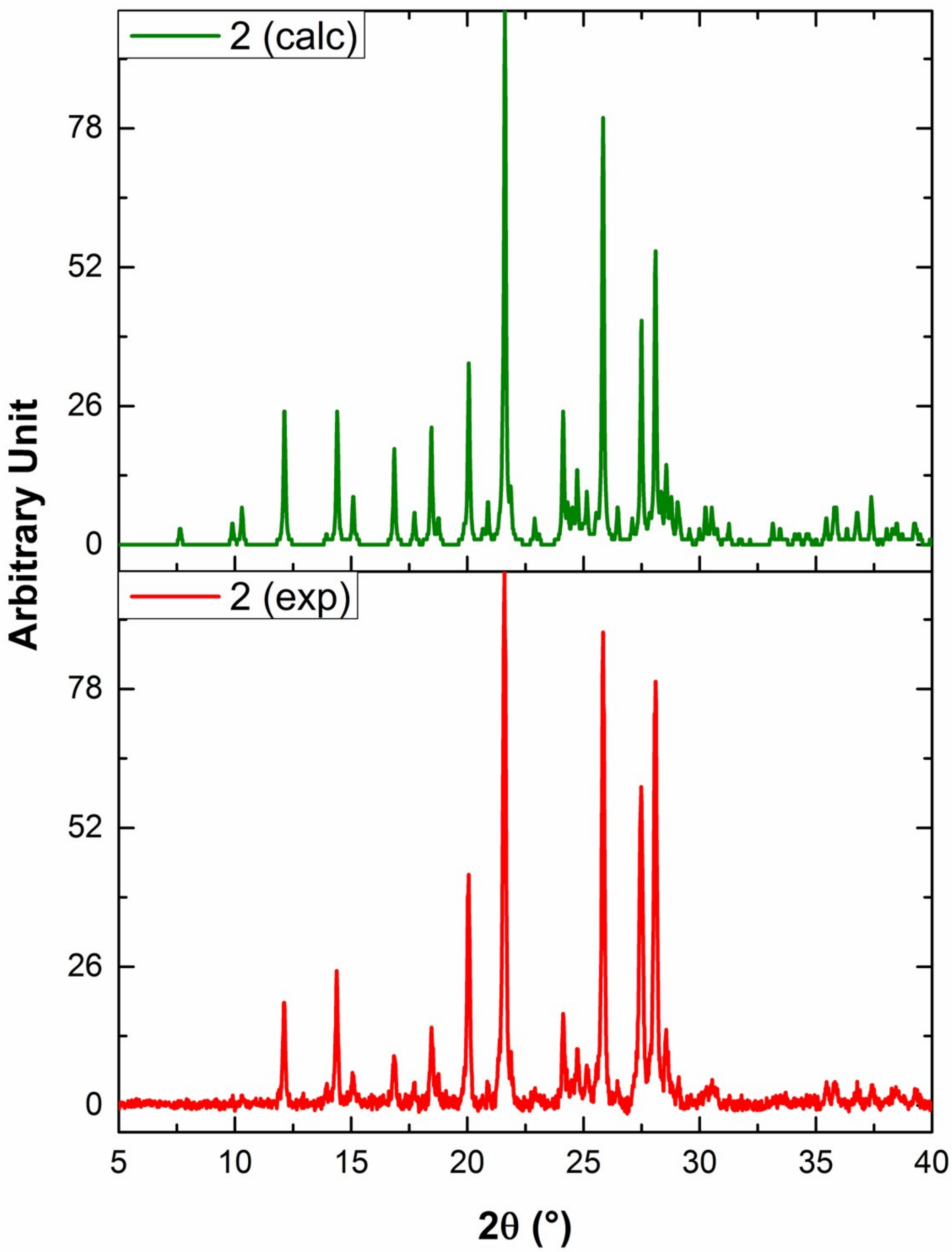


Figure S18. Comparative PXRD patterns simulated (top) and experimental for compound **2** (bottom).



2 (calc)
2 (exp)
Arbitrary Unit
0
26
52
78
5
10
15
20
25
30
35
40
2θ (°)

Figure S19. Comparative PXRD patterns simulated (top) and experimental for compound **3** (bottom).

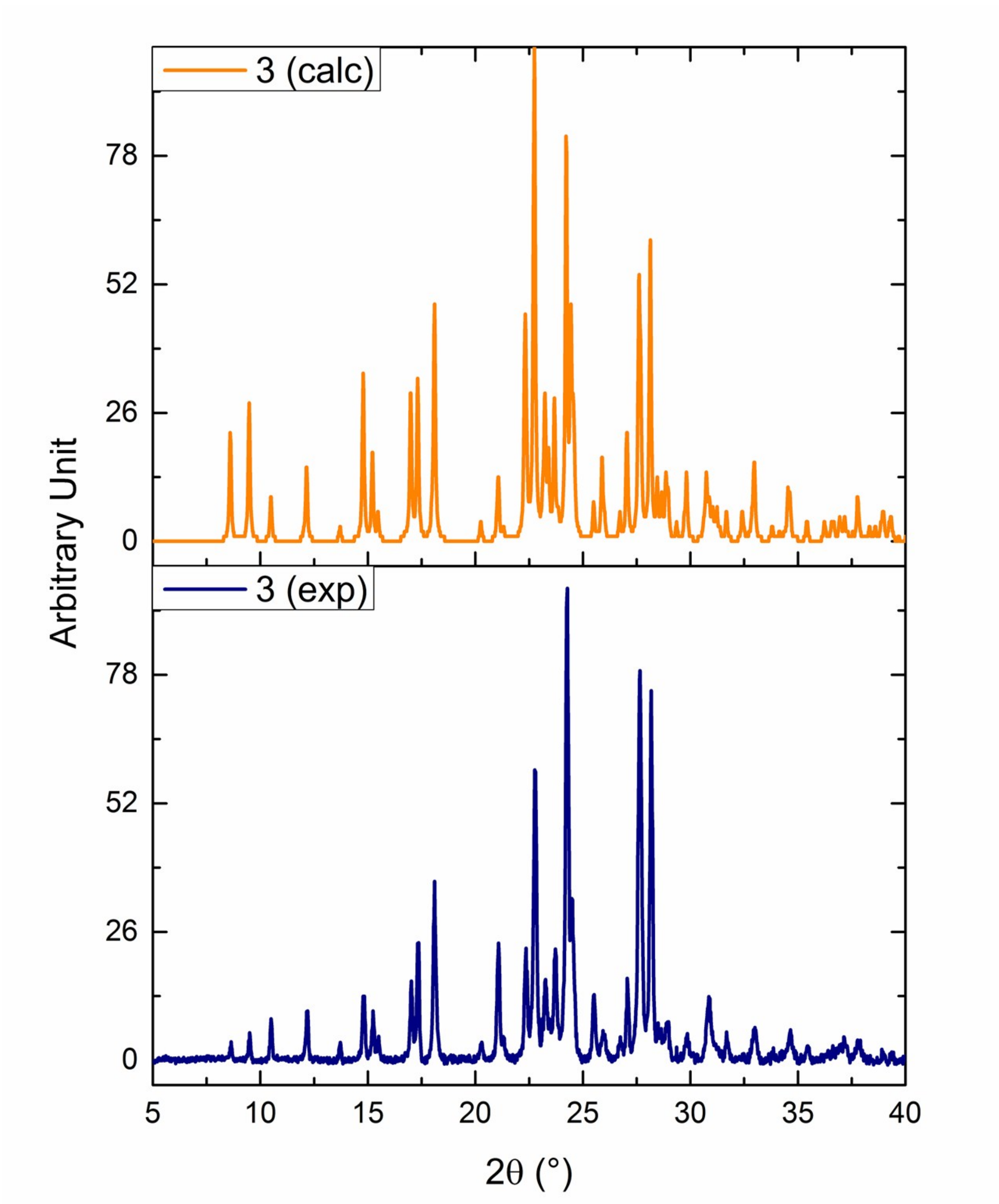


Figure S20. Comparative PXRD patterns simulated (top) and experimental for compound **4** (bottom).

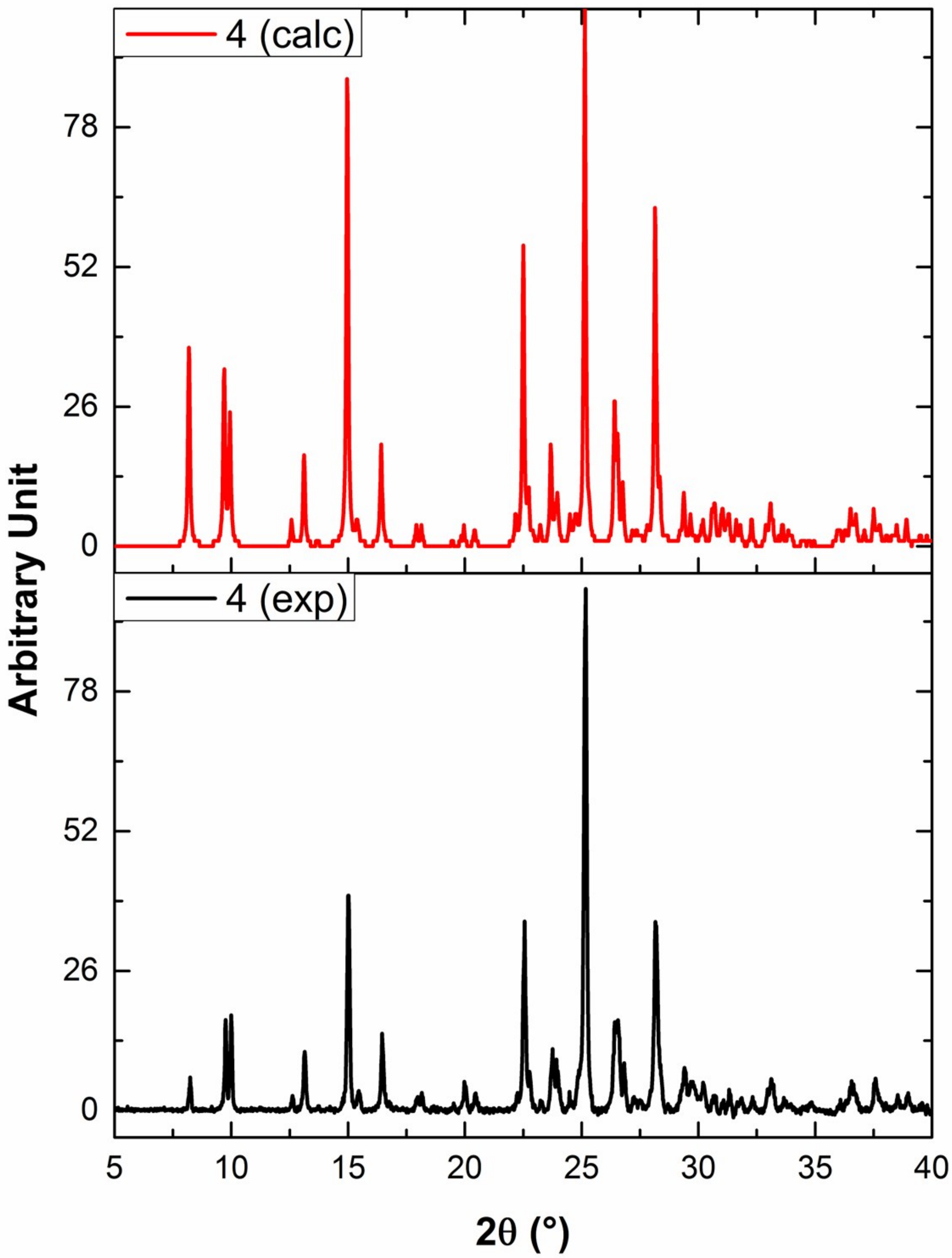


Figure S21. Comparative PXRD patterns simulated (top) and experimental for compound **5** (bottom).

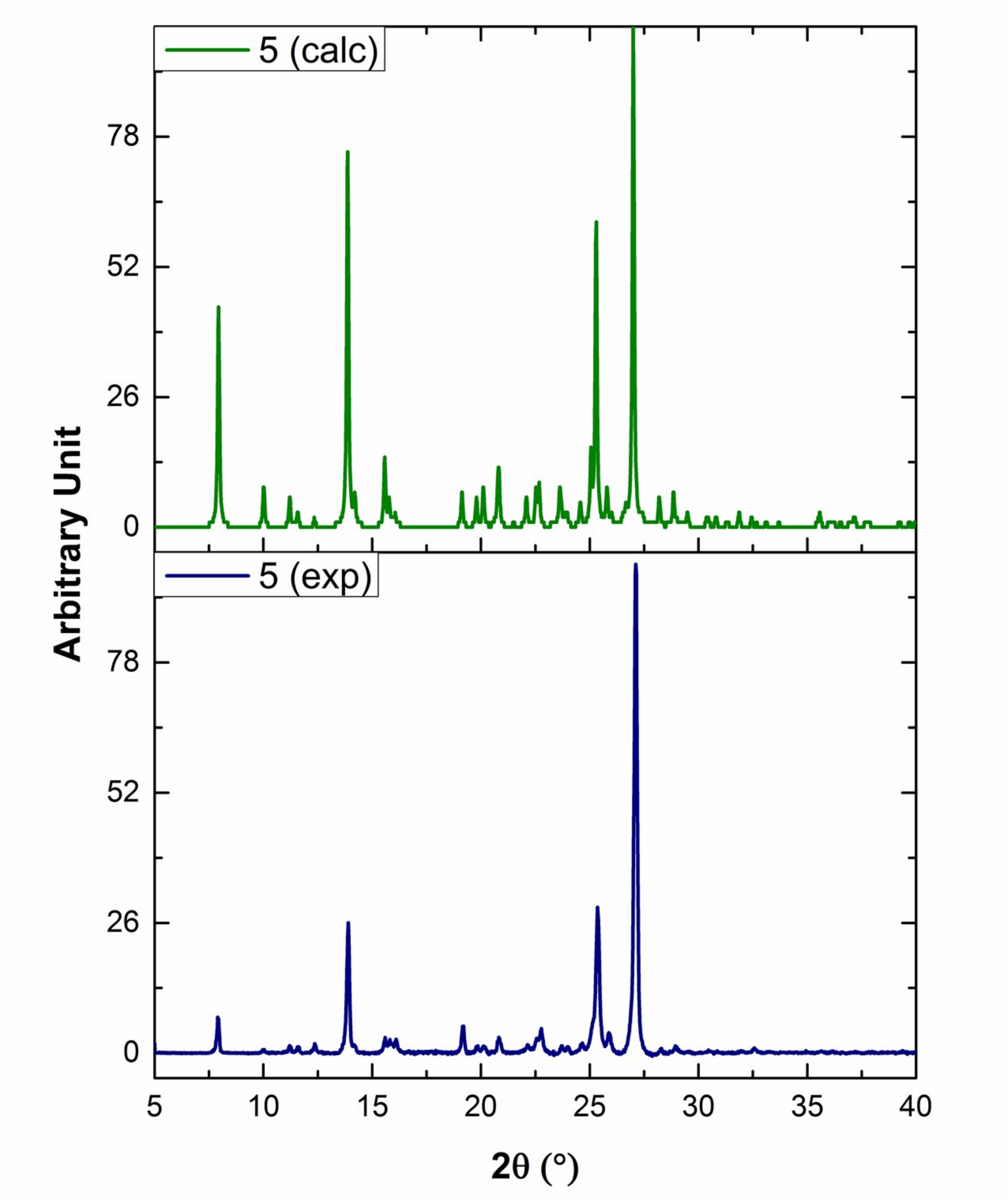


Figure S22. Comparative PXRD patterns simulated (top) and experimental for compound **6** (bottom).

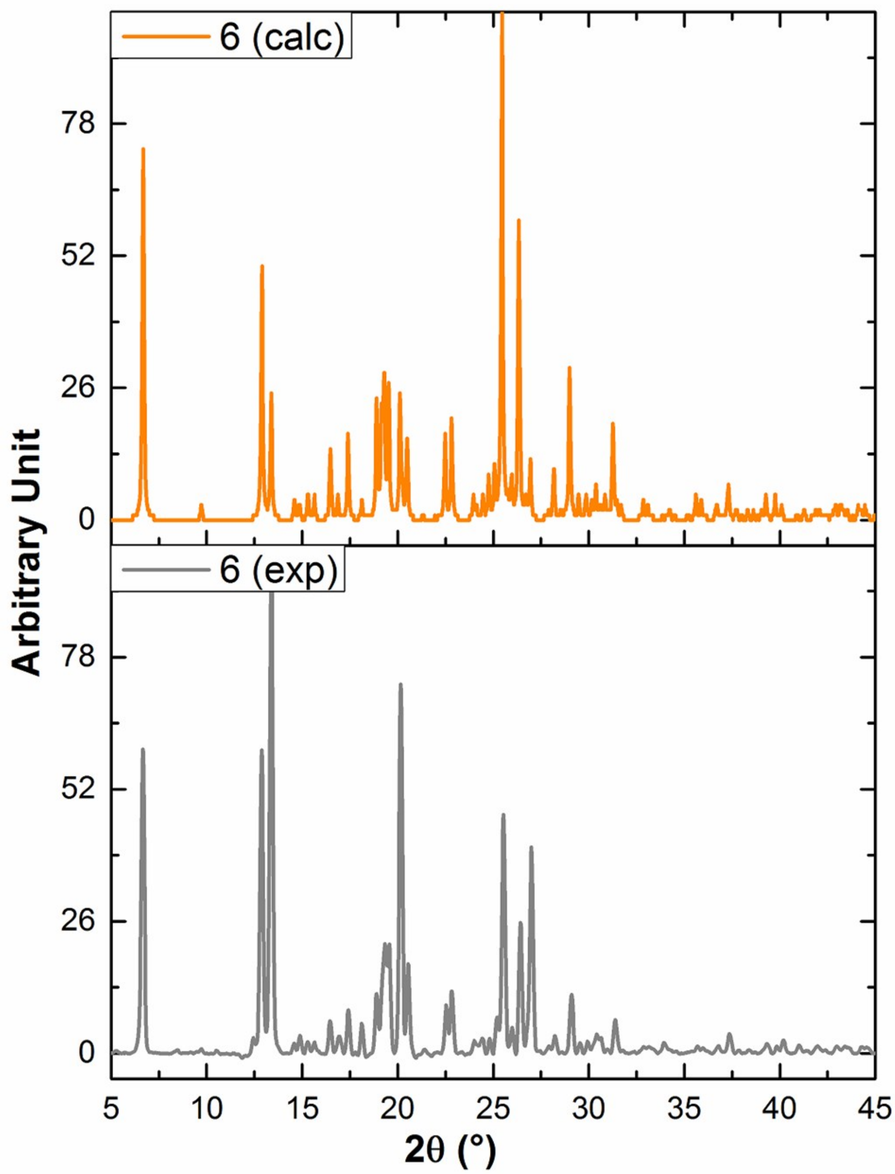


Figure S23. From bottom to top: Comparative PXRD patterns simulated and experimental for compounds **7** and **8**.

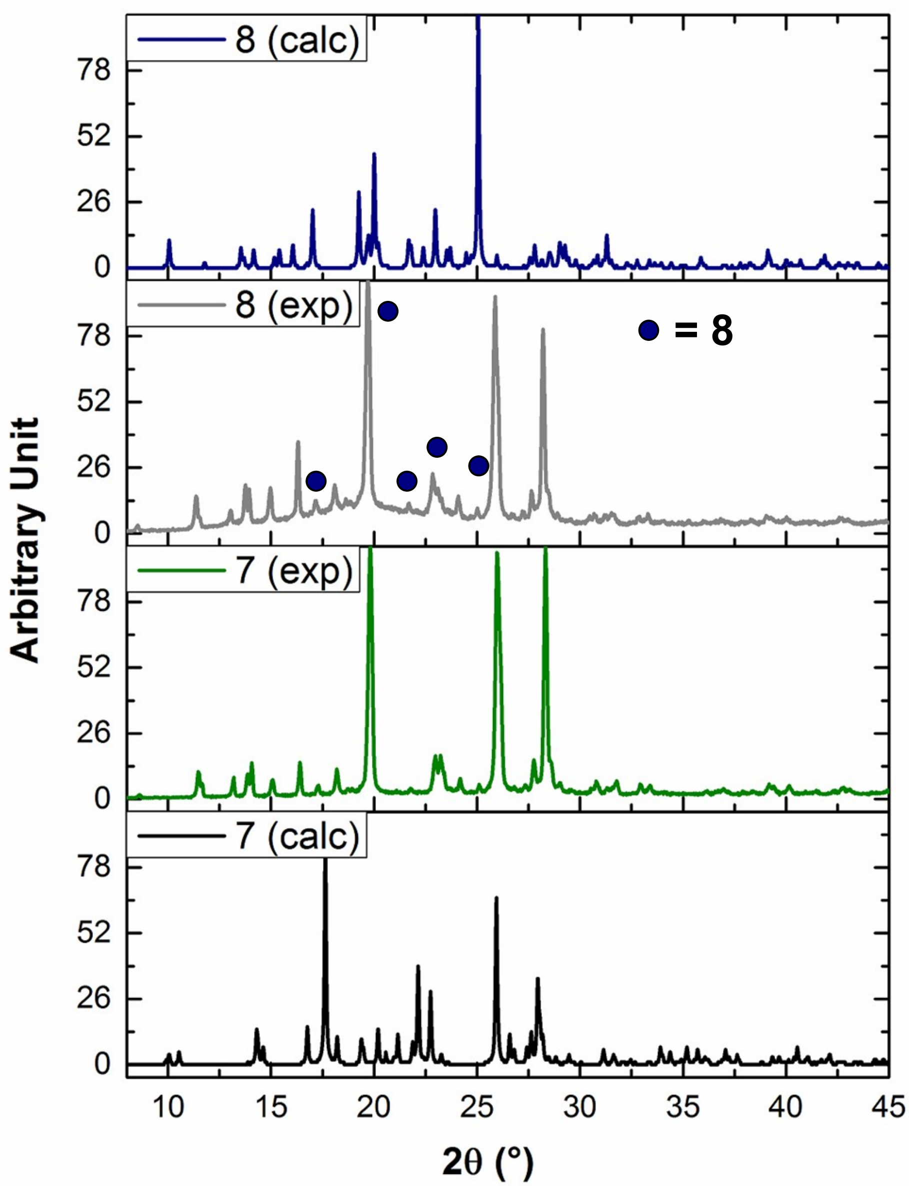


Figure S24. Comparative PXRD patterns simulated (top) and experimental for compound **9** (bottom).

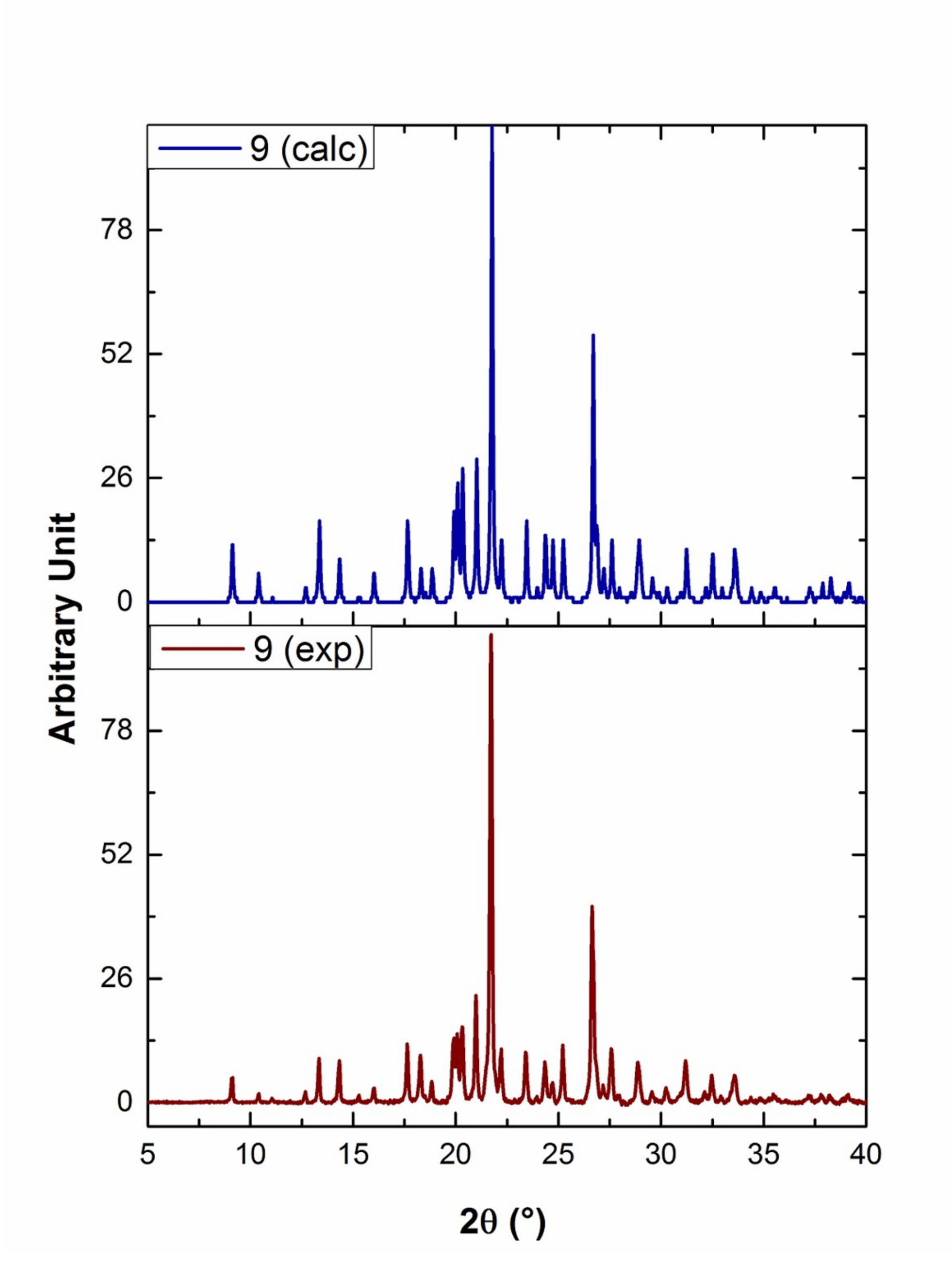


Figure S25. Comparative PXRD patterns simulated (top) and experimental for compound **10** (bottom).