Supporting Information

One Dimensional Halogen Bond Design: Br···N versus I···N with Fluoroarenes

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Cocrystal synthesis

(Br_2F_4bz)(Me_2pyrz): In a 20 mL glass vial, 1,4-dibromotetrafluorobenzene (91 mg, 0.30 mmol) and 2,5-dimethylpyrazine (0.032 mL, 0.30 mmol) were combined in ethanol (5 mL) and vigorously stirred until all solids had dissolved. The solvent was then allowed to slowly evaporate under ambient conditions until crystalline material was observed. The vial was then sealed to cease evaporation and preserve sample purity. T_{decomp} 87°C. Anal Calcd for $C_{12}H_8Br_2F_4N_2$ (416.01): C, 34.65; H, 1.94; N, 6.73; Found: C, 34.97; H, 2.27; N, 7.06.

(I_2F_4bz)(Me_2pyrz): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 1,4-diiodotetrafluorobenzene (87 mg, 0.22 mmol) and 2,5-dimethylpyrazine (0.024 mL, 0.22 mmol) dissolved in ethanol. T_{decomp} 131°C. Anal Calcd for $C_{12}H_8F_4I_2N_2$ (510.01): C, 28.26; H, 1.58; N, 5.49; Found: C, 27.95; H, 1.42; N, 5.64.

(Br_2F_8bph)(Me_2pyrz): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 4,4'-dibromooctafluorobenzene (82 mg, 0.18 mmol) and 2,5-dimethylpyrazine (0.020 mL, 0.18 mmol) dissolved in ethanol. T_{decomp} 101°C. Anal Calcd for $C_{18}H_8Br_2F_8N_2$ (564.07): C, 38.33; H, 1.43; N, 4.97; Found: C, 38.12; H, 1.74; N, 4.57.

(I_2F_8bph)(Me_2pyrz): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 4,4'-diiodooctafluorobenzene (93 mg, 0.17 mmol) and 2,5-dimethylpyrazine (0.018 mL, 0.17 mmol) dissolved in ethanol. T_{decomp} 200°C. Anal Calcd for $C_{18}H_8F_8I_2N_2$ (658.07): C, 32.85; H, 1.23; N, 4.26; Found: C, 32.49; H, 1.18; N, 4.34.

(I_2F_4bz)(Me_3pyrz): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 1,4-diiodotetrafluorobenzene (90 mg, 0.22 mmol) and 2,5-dimethylpyrazine (0.028 mL, 0.22 mmol) dissolved in ethanol. T_{decomp} 139°C. Anal Calcd for $C_{13}H_{10}F_4I_2N_2$ (524.04): C, 29.80; H, 1.92; N, 5.35; Found: C, 29.92; H, 2.24; N, 5.09.

(Br_2F_4bz)(Me_4pyrz)$_2$: A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 1,4-dibromotetrafluorobenzene (67 mg, 0.22 mmol) and 2,3,5,6-tetramethylpyrazine (59 mg, 0.44 mmol) dissolved in ethanol. Reactions conducted at 1:1 stoichiometry also produced a 1:2 cocrystal. T_{decomp} 101°C. Anal Calcd for $C_{22}H_{24}Br_2F_4N_4$ (580.26): C, 45.54; H, 4.17; N, 9.66; Found: C, 45.94; H, 4.11; N, 9.87.

(Br_2F_8bph)(Me_4pyrz): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 4,4'-dibromooctafluorobenzene (97 mg, 0.21 mmol) and 2,3,5,6-tetramethylpyrazine (29 mg, 0.21 mmol) dissolved in ethanol. T_{decomp} 126°C. Anal Calcd for $C_{20}H_{12}Br_2F_8N_2$ (592.13): C, 40.57; H, 2.04; N, 4.73; Found: C, 40.54; H, 2.21; N, 4.69.

(I_2F_8bph)(Me_4pyrz): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 4,4'-diiodooctafluorobenzene (92 mg, 0.30 mmol) and 2,3,5,6-tetramethylpyrazine (41 mg, 0.30 mmol) dissolved in ethanol. T_{decomp} 203°C. Anal Calcd for $C_{20}H_{12}F_8I_2N_2$ (686.13): C, 35.01; H, 1.76; N, 4.08; Found: C, 35.38; H, 1.93; N, 4.40.

(Br_2F_4bz)(quinox): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 1,4-dibromotetrafluorobenzene (85 mg, 0.28 mmol) and quinoxaline (36 mg,

0.28 mmol) dissolved in ethanol. T_{decomp} 116°C. Anal Calcd for $C_{14}H_6Br_2F_4N_2$ (438.02): C, 38.39; H, 1.38; N, 6.40; Found: C, 38.36; H, 1.31; N, 6.24.

(Br_2F_8bph)(quinox): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 4,4'-dibromooctafluorobenzene (99 mg, 0.22 mmol) and quinoxaline (28 mg, 0.22 mmol) dissolved in ethanol. T_{decomp} 117°C. Anal Calcd for $C_{20}H_6Br_2F_8N_2$ (586.08): C, 20.99; H, 1.03; N, 4.78; Found: C, 21.19; H, 0.93; N, 4.99.

(I_2F_8bph)(quinox): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 4,4'-diiodooctafluorobenzene (101 mg, 0.18 mmol) and quinoxaline (24 mg, 0.18 mmol) dissolved in ethanol. T_{decomp} 146°C. Anal Calcd for $C_{20}H_6F_8I_2N_2$ (680.08): C, 35.32; H, 0.89; N, 4.12; Found: C, 35.05; H, 0.57; N, 4.47.

(Br_2F_8bph)(phenaz): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 4,4'-dibromooctafluorobenzene (92 mg, 0.20 mmol) and phenazine (36 mg, 0.20 mmol) dissolved in ethanol. T_{decomp} 156°C. Anal Calcd for $C_{24}H_8Br_2F_8N_2$ (636.14): C, 45.32; H, 1.27; N, 4.40; Found: C, 45.38; H, 1.59; N, 4.43.

(I_2F_8bph)(phenaz): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 4,4'-diiodooctafluorobenzene (106 mg, 0.19 mmol) and phenazine (35 mg, 0.19 mmol) dissolved in ethanol. T_{decomp} 181°C. Anal Calcd for $C_{24}H_8F_8I_2N_2$ (730.14): C, 39.48; H, 1.10; N, 3.84; Found: C, 39.47; H, 1.15; N, 3.98.

(Br_2F_4bz)(2,2'-bipy): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 1,4-dibromotetrafluorobenzene (86 mg, 0.28 mmol) and 2,2'-bipyridine (44 mg, 0.28 mmol) dissolved in ethanol. T_{decomp} 200°C. Anal Calcd for $C_{16}H_8Br_2F_4N_2$ (464.06): C, 41.41; H, 1.74; N, 6.04; Found: C, 41.79; H, 1.61; N, 6.14.

(Br_2F_8bph)(2,2'-bipy): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 4,4'-dibromooctafluorobenzene (108 mg, 0.24 mmol) and 2,2'-bipyridine (37 mg, 0.24 mmol) dissolved in ethanol. T_{decomp} 149°C. Anal Calcd for $C_{44}H_{16}Br_4F_{16}N_4$ (1224.23): C, 43.17; H, 1.32; N, 4.58; Found: C, 43.21; H, 1.08; N, 4.42.

(I_2F_8bph)(2,2'-bipy): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 4,4'-diiodooctafluorobenzene (109 mg, 0.20 mmol) and 2,2'-bipyridine (31 mg, 0.20 mmol) dissolved in ethanol. T_{decomp} 209°C. Anal Calcd for $C_{22}H_8F_8I_2N_2$ (581.12): C, 37.42; H, 1.14; N, 3.97; Found: C, 37.31; H, 1.24; N, 3.65.

(Br_2F_4bz)(Me_2-2,2'-bipy): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 1,4-dibromotetrafluorobenzene (94 mg, 0.31 mmol) and 4,4'-dimethyl-2,2'-bipyridine (56 mg, 0.31 mmol) dissolved in ethanol. T_{decomp} 78°C. Anal Calcd for $C_{18}H_{12}Br_2F_4N_2$ (492.11): C, 23.93; H, 2.46; N, 5.69; Found: C, 23.94; H, 2.56; N, 5.51.

(I_2F_4bz)(Me_2-2,2'-bipy): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 1,4-diiodotetrafluorobenzene (98 mg, 0.24 mmol) and 4,4'-dimethyl-2,2'-bipyridine (45 mg, 0.24 mmol) dissolved in ethanol. T_{decomp} 103°C. Anal Calcd for $C_{18}H_{12}F_4I_2N_2$ (586.11): C, 36.89; H, 2.06; N, 4.78; Found: C, 37.17; H, 2.00; N, 4.77.

(Br_2F_8bph)(Me_2-2,2'-bipy): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 4,4'-dibromooctafluorobenzene (96 mg, 0.21 mmol) and 4,4'-dimethyl-2,2'-bipyridine (39 mg, 0.21 mmol) dissolved in ethanol. T_{decomp} 147°C. Anal Calcd for $C_{24}H_{12}Br_2F_8N_2$ (640.17): C, 45.03; H, 1.89; N, 4.38; Found: C, 45.18; H, 1.95; N, 4.03.

(I_2F_8bph)(Me_2-2,2'-bipy): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 4,4'-diiodooctafluorobenzene (86 mg, 0.16 mmol) and 4,4'-dimethyl-2,2'-bipyridine (29 mg, 0.16 mmol) dissolved in ethanol. T_{decomp} 160°C. Anal Calcd for $C_{24}H_{12}F_8I_2N_2$ (734.17): C, 39.10; H, 1.65; N, 3.82; Found: C, 39.10; H, 1.35; N, 3.71.

(Br_2F_8bph)(4,4'-bipy): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 4,4'-dibromooctafluorobenzene (95 mg, 0.21 mmol) and 4,4'-bipyridine (33 mg, 0.21 mmol) dissolved in ethanol. T_{decomp} 162°C. Anal Calcd for $C_{22}H_8Br_2F_8N_2$ (612.12): C, 43.17; H, 1.32; N, 4.58; Found: C, 43.44; H, 1.62; N, 4.83.

(I_2F_8bph)(4,4'-bipy): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 4,4'-diiodooctafluorobenzene (80 mg, 0.15 mmol) and 4,4'-bipyridine (23 mg, 0.15 mmol) dissolved in ethanol. T_{decomp} 206°C. Anal Calcd for $C_{22}H_8F_8I_2N_2$ (706.12): C, 37.42; H, 1.14; N, 3.97; Found: C, 37.72; H, 1.26; N, 4.19.

(Br_2F_8bph)(dpe): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 4,4'-dibromooctafluorobenzene (91 mg, 0.20 mmol) and 1,2-di(4-pyridyl)ethylene (36 mg, 0.20 mmol) dissolved in ethanol. T_{decomp} 155°C. Anal Calcd for $C_{24}H_{10}Br_2F_8N_2$ (638.15): C, 45.17; H, 1.58; N, 4.39; Found: C, 44.80; H, 1.60; N, 4.72.

(Br_2F_8bph)$_2$(dpe): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 4,4'-dibromooctafluorobenzene (97 mg, 0.43 mmol) and 1,2-di(4-pyridyl)ethylene (19 mg, 0.21 mmol) dissolved in ethanol. T_{decomp} 184°C. Anal Calcd for $C_{24}H_{10}F_8I_2N_2$ (732.16): C, 39.37; H, 1.38; N, 3.83; Found: C, 39.59; H, 1.77; N, 3.84.

(I_2F_8bph)(dpe): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 4,4'-diiodooctafluorobenzene (110 mg, 0.20 mmol) and 1,2-di(4-pyridyl)ethylene (36 mg, 0.20 mmol) dissolved in ethanol. T_{decomp} 175°C. Anal Calcd for $C_{24}H_{10}F_8I_2N_2$ (732.16): C, 39.37; H, 1.38; N, 3.83; Found: C, 39.59; H, 1.77; N, 3.84.

(Br_2F_8bph)(DABCO): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 4,4'-dibromooctafluorobenzene (85 mg, 0.19 mmol) and 1,4-diazabicyclo[2.2.2]octane (21 mg, 0.19 mmol) dissolved in a 1:1 mixture of ethanol:dichloromethane. T_{decomp} 173°C. Anal Calcd for $C_{18}H_{12}Br_2F_8N_2$ (568.10): C, 38.06; H, 2.13; N, 4.93; Found: C, 38.12; H, 1.76; N, 5.04.

(I_2F_8bph)(DABCO): A crystalline sample was obtained according to the same general procedure as (Br_2F_4bz)(Me_2pyrz), utilizing 4,4'-diiodooctafluorobenzene (83 mg, 0.24 mmol) and 1,4-diazabicyclo[2.2.2]octane (27 mg, 0.24 mmol) dissolved in a 1:1 mixture of ethanol:dichloromethane.. T_{decomp} 200°C. Anal Calcd for $C_{18}H_{12}F_8I_2N_2$ (662.11): C, 32.65; H, 1.83; N, 4.23; Found: C, 32.92; H, 1.70; N, 4.36.

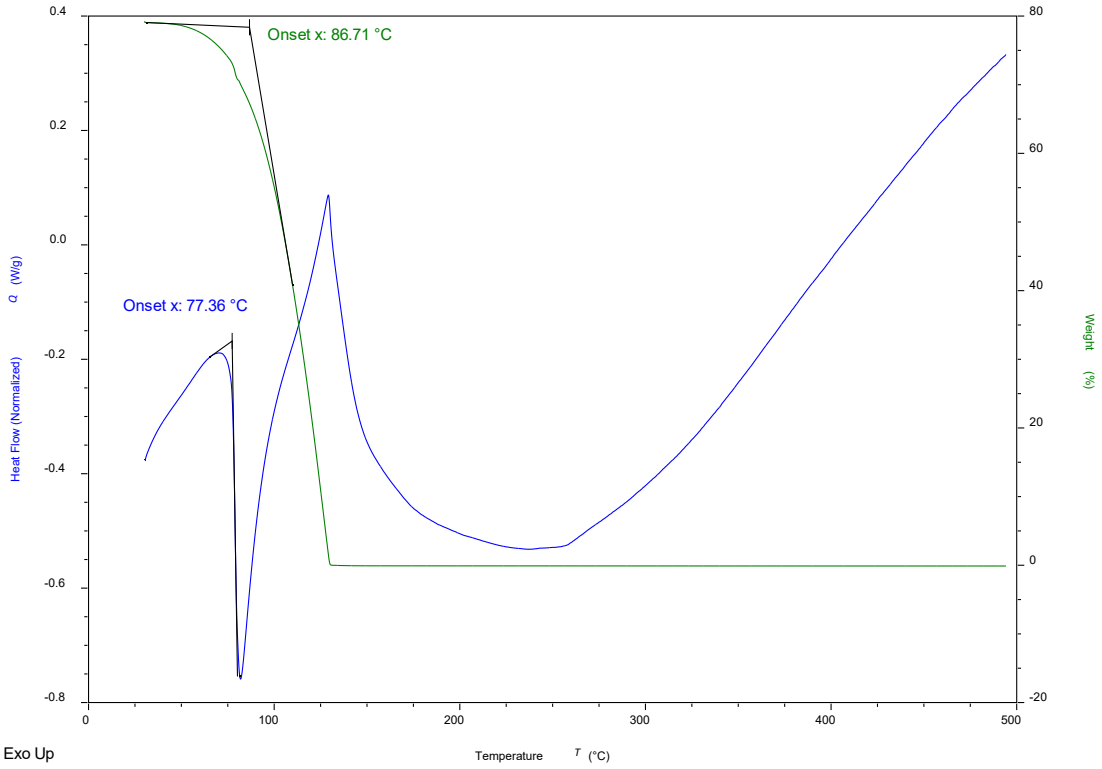

Figure SI1. SDT of $(Br_2F_4bz)(Me_2pyrz)$

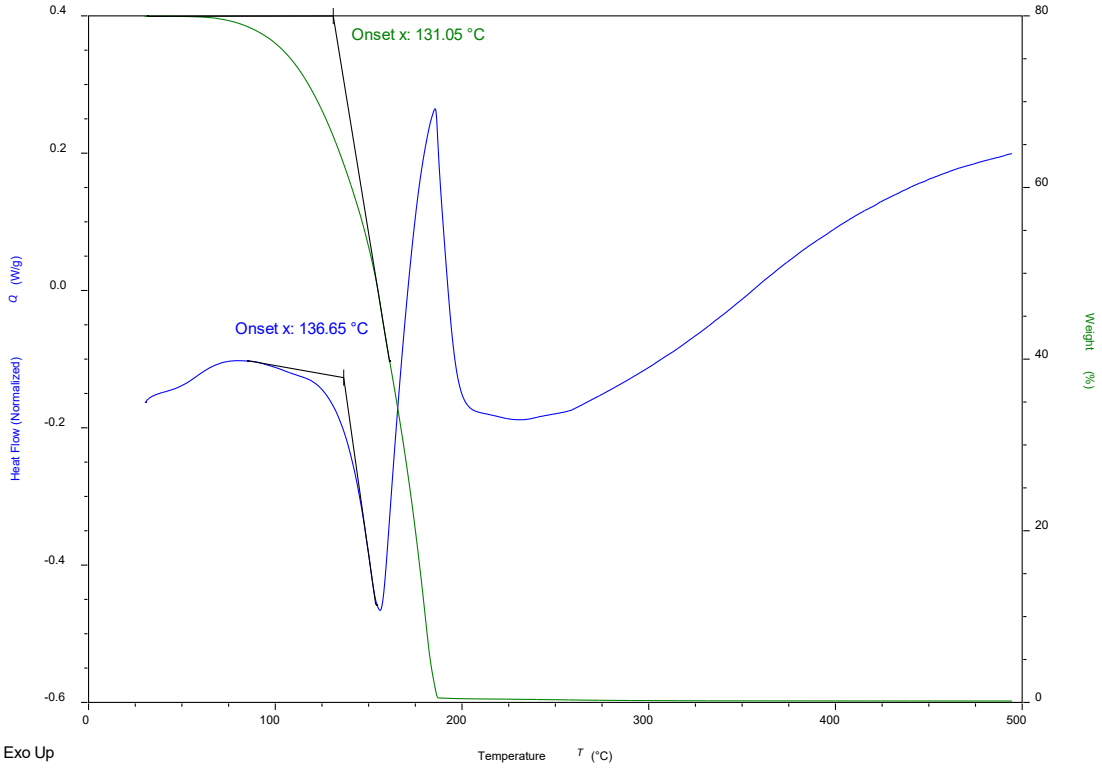

Figure SI2. SDT of $(I_2F_4bz)(Me_2pyrz)$

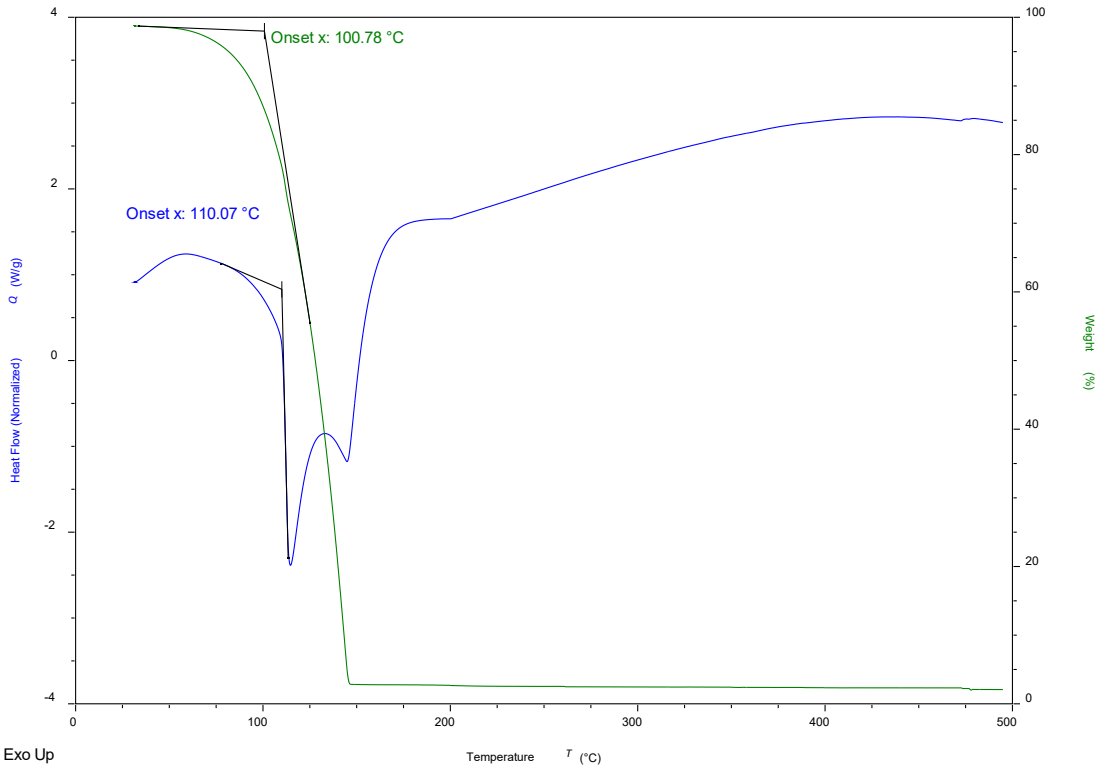

Figure SI3. SDT of (Br_2F_8bph)(Me_2pyrz)

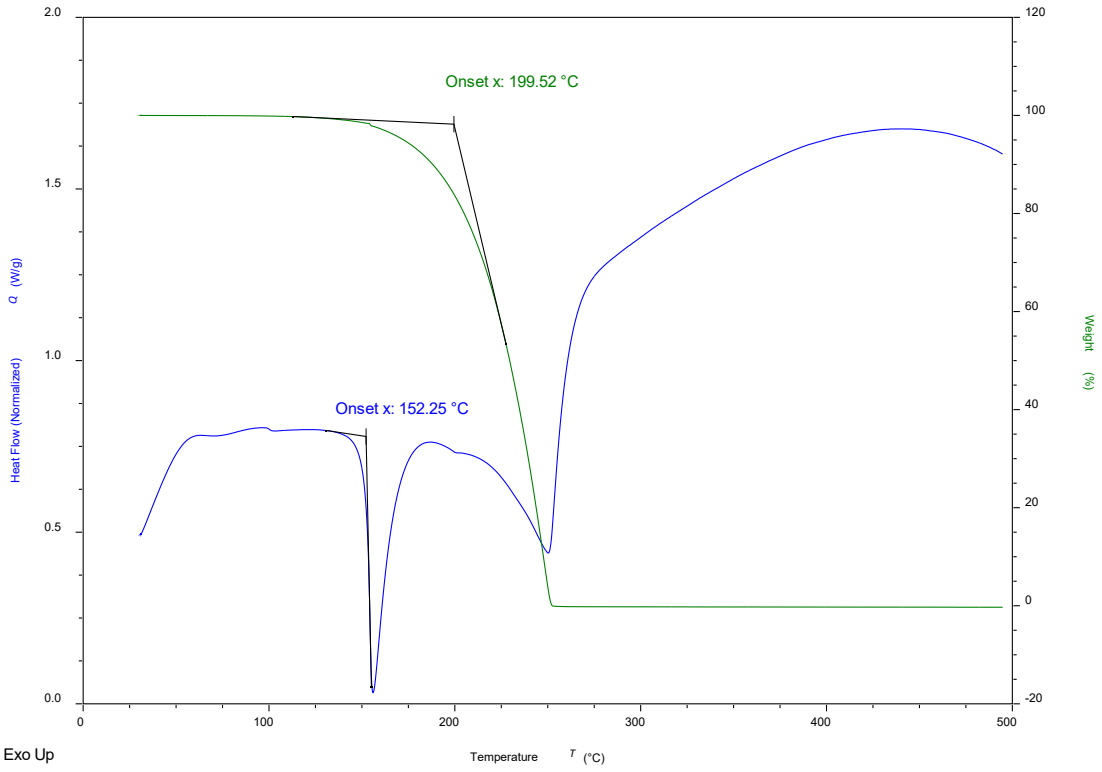

Figure SI4. SDT of (I_2F_8bph)(Me_2pyrz)

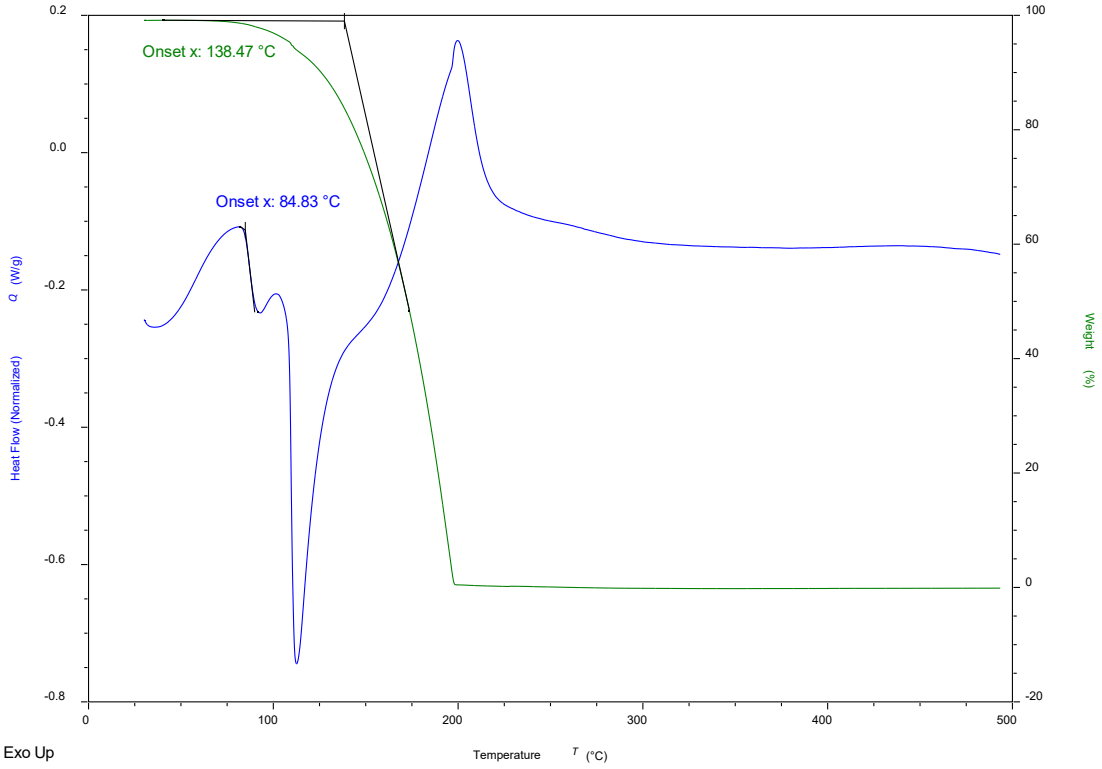

Figure SI5. SDT of $(I_2F_4bz)(Me_3pyrz)$

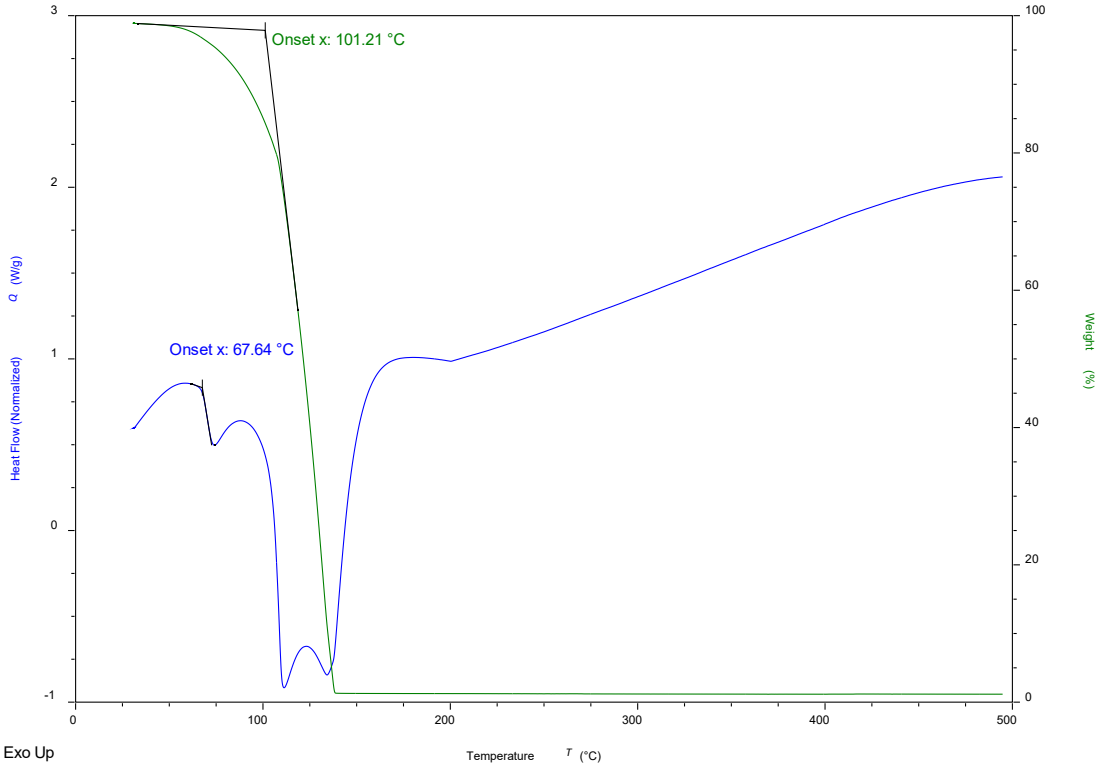

Figure SI6. SDT of $(Br_2F_4bz)(Me_4pyrz)_2$

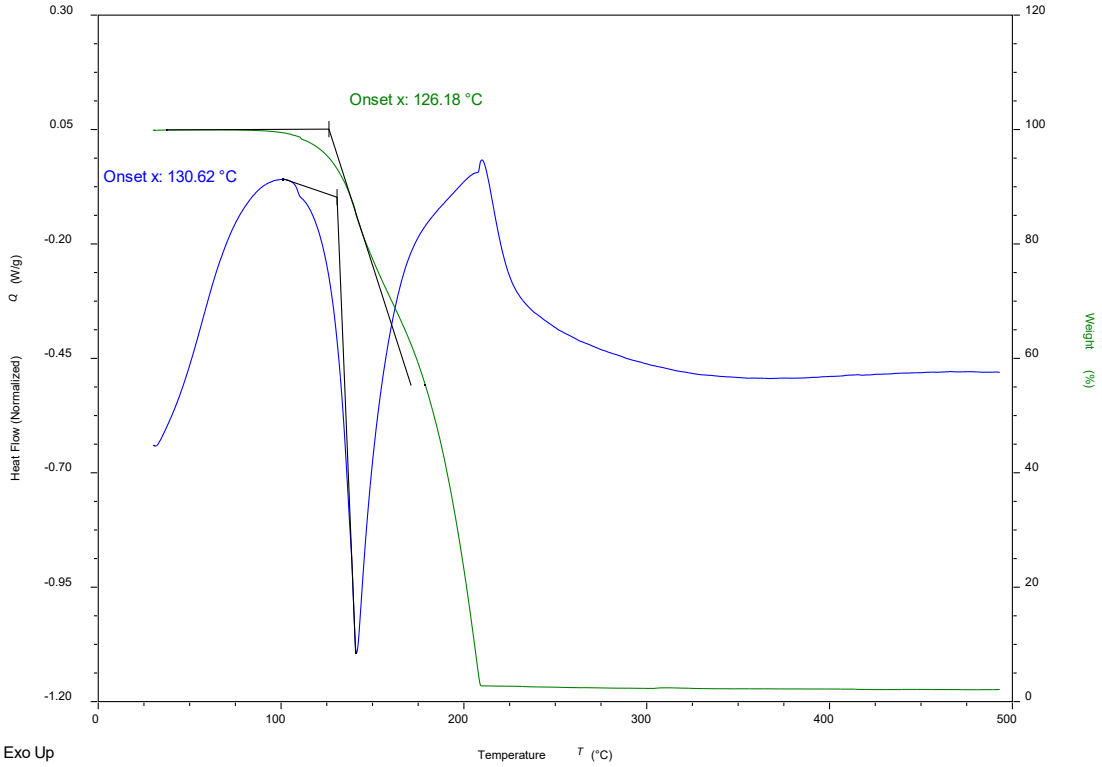

Figure SI7. SDT of (Br_2F_8bph)(Me_4pyrz)

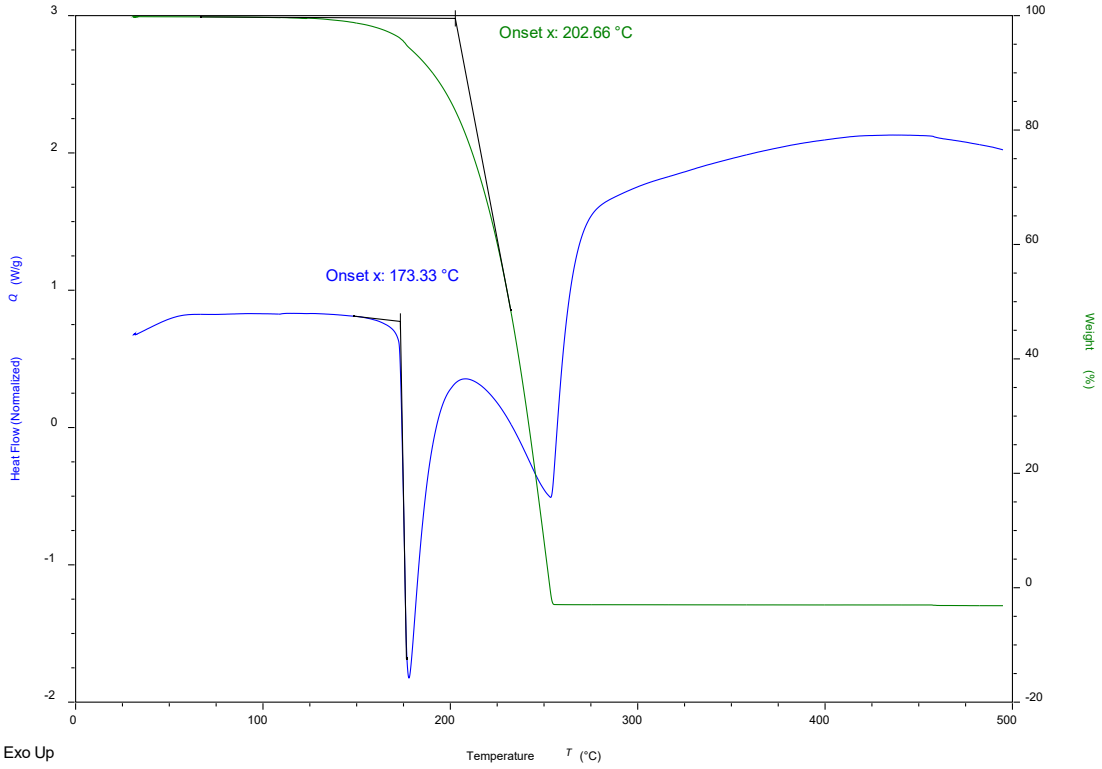

Figure SI8. SDT of (I_2F_8bph)(Me_4pyrz)

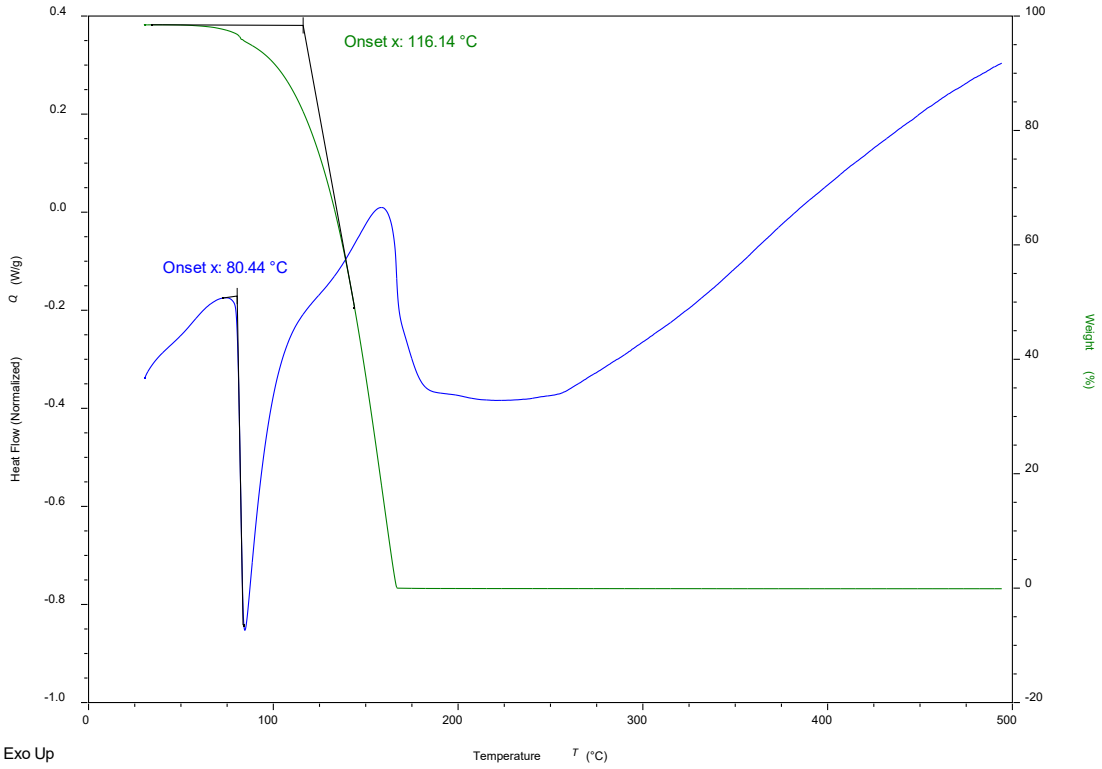

Figure SI9. SDT of (Br_2F_4bz)(quinox)

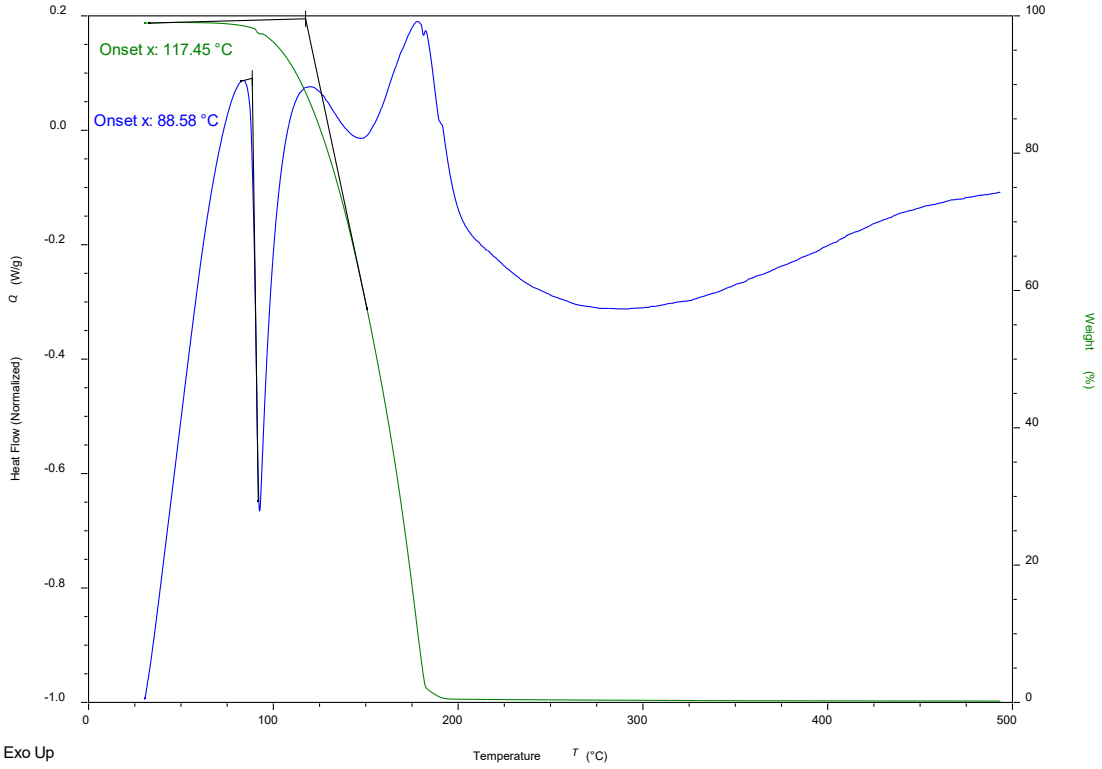

Figure SI10. SDT of (Br_2F_8bph)(quinox)

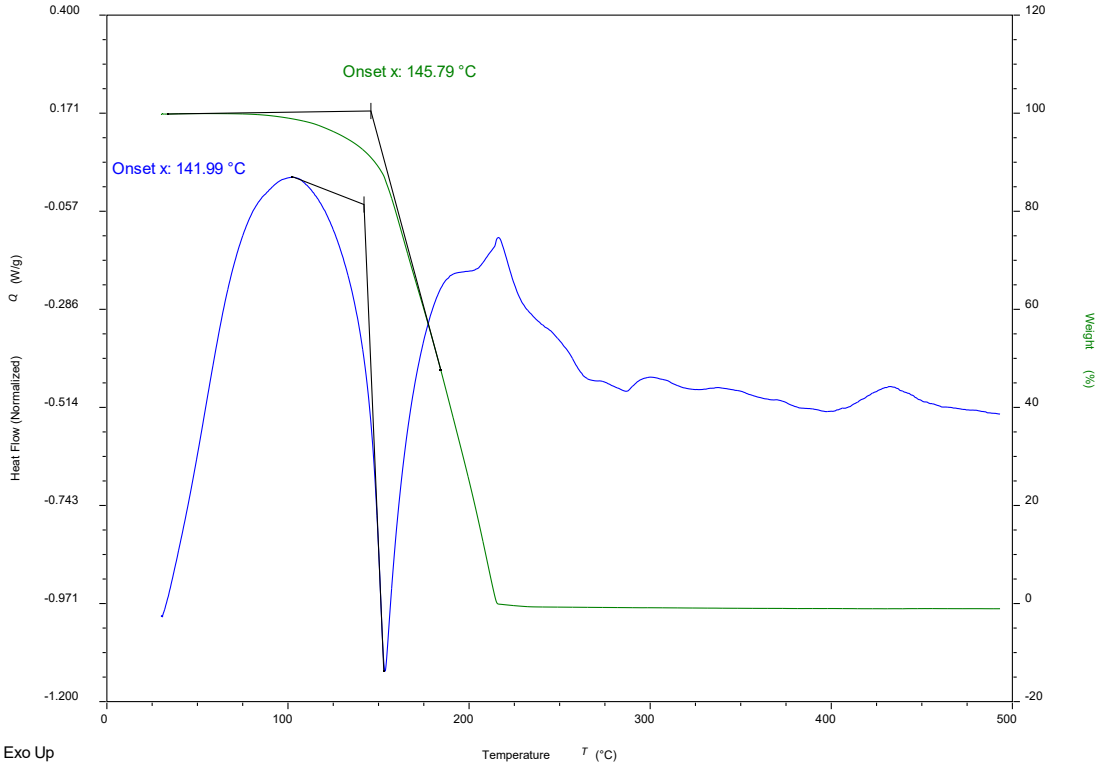

Figure SI11. SDT of (I_2F_8bph)(quinox)

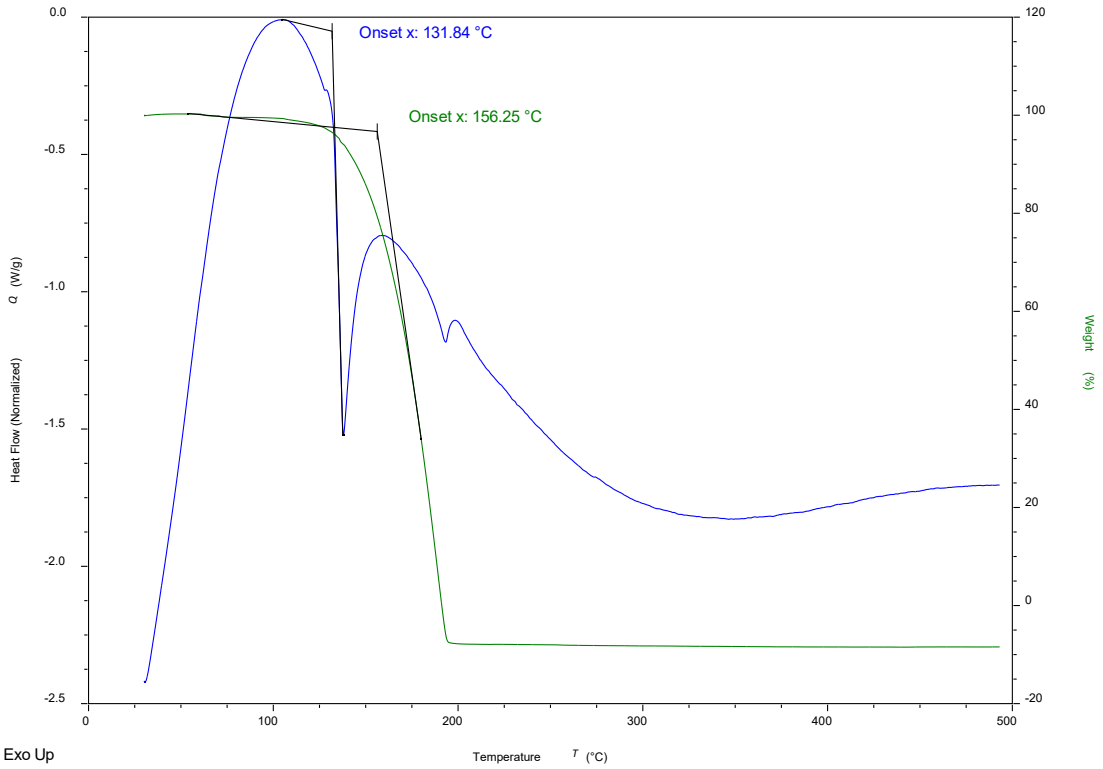

Figure SI12. SDT of (Br_2F_8bph)(phenaz)

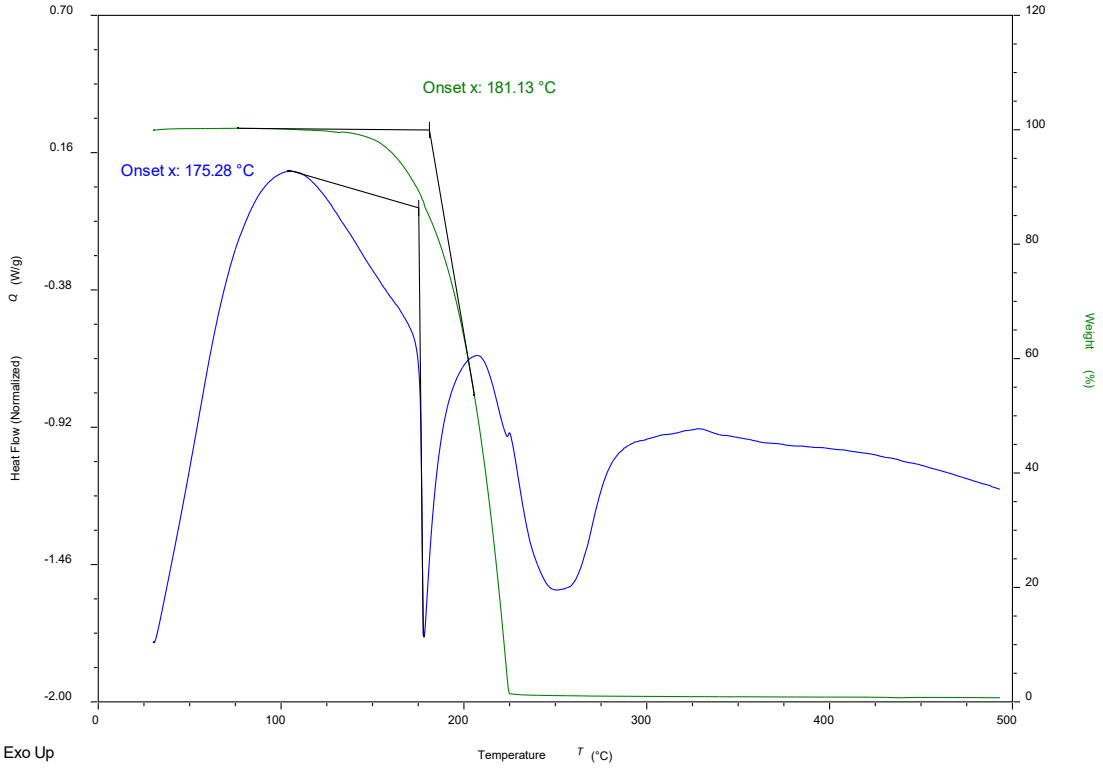

Figure SI13. SDT of (I_2F_8bph)(phenaz)

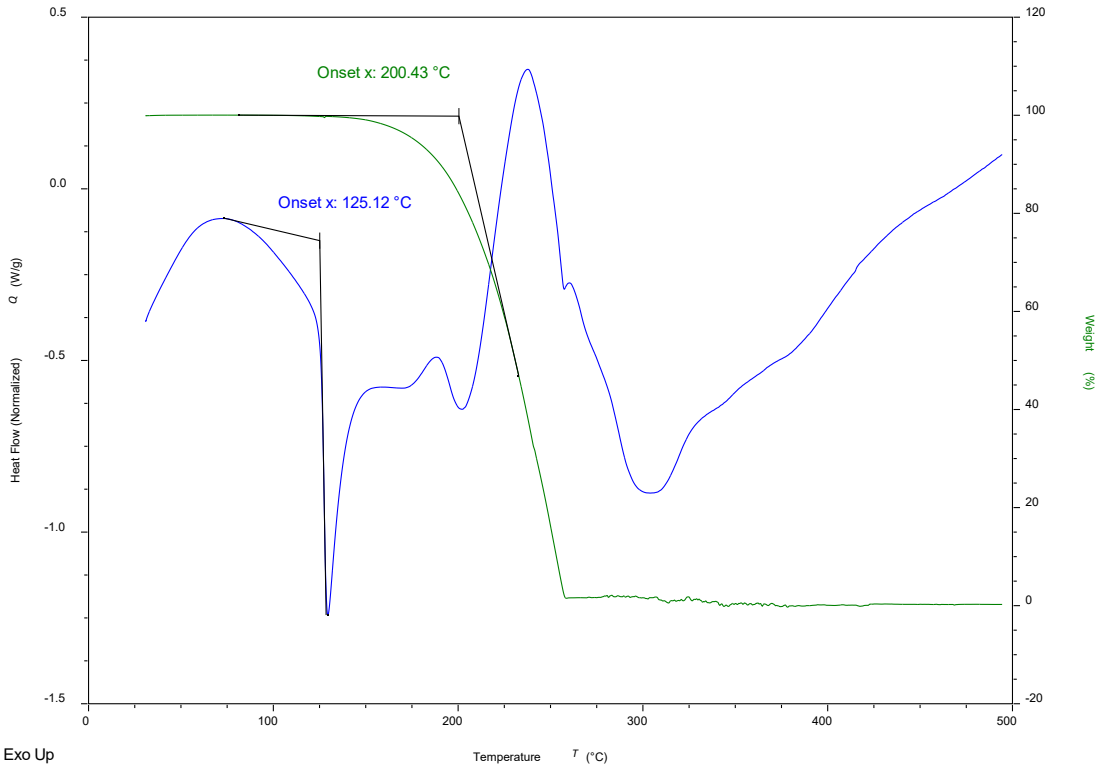

Figure SI14. SDT of (Br_2F_4bz)(2,2'-bipy)

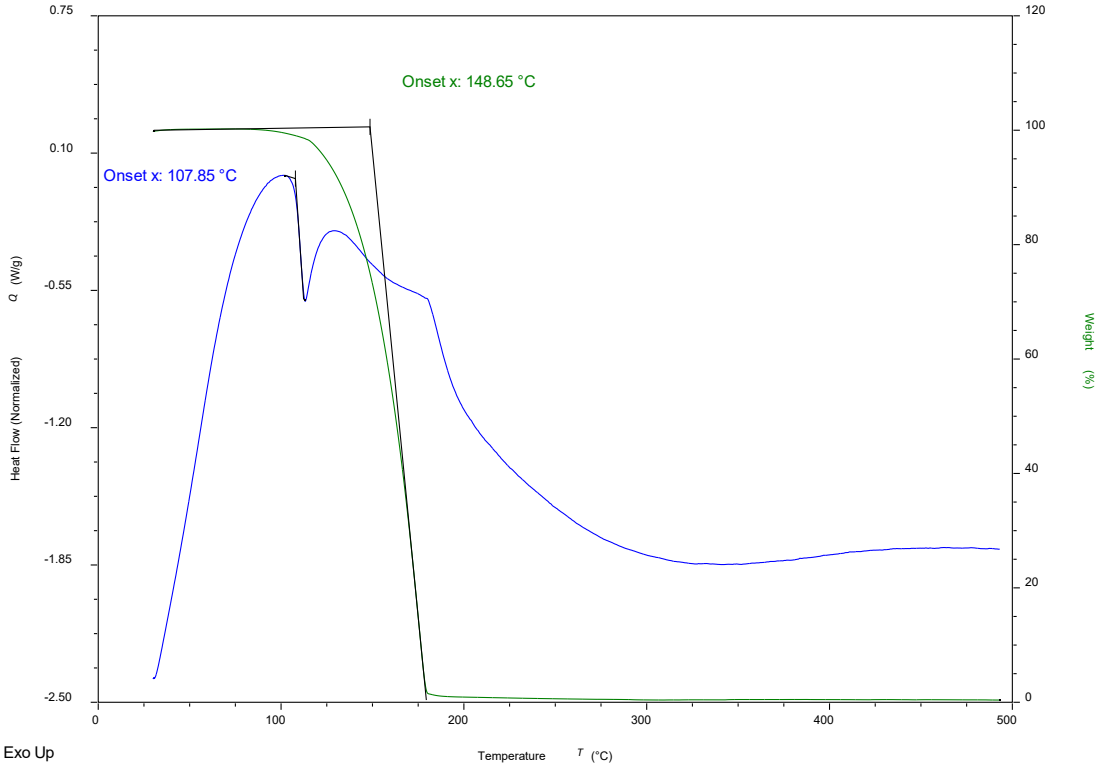

Figure SI15. SDT of (Br_2F_8bph)(2,2'-bipy)

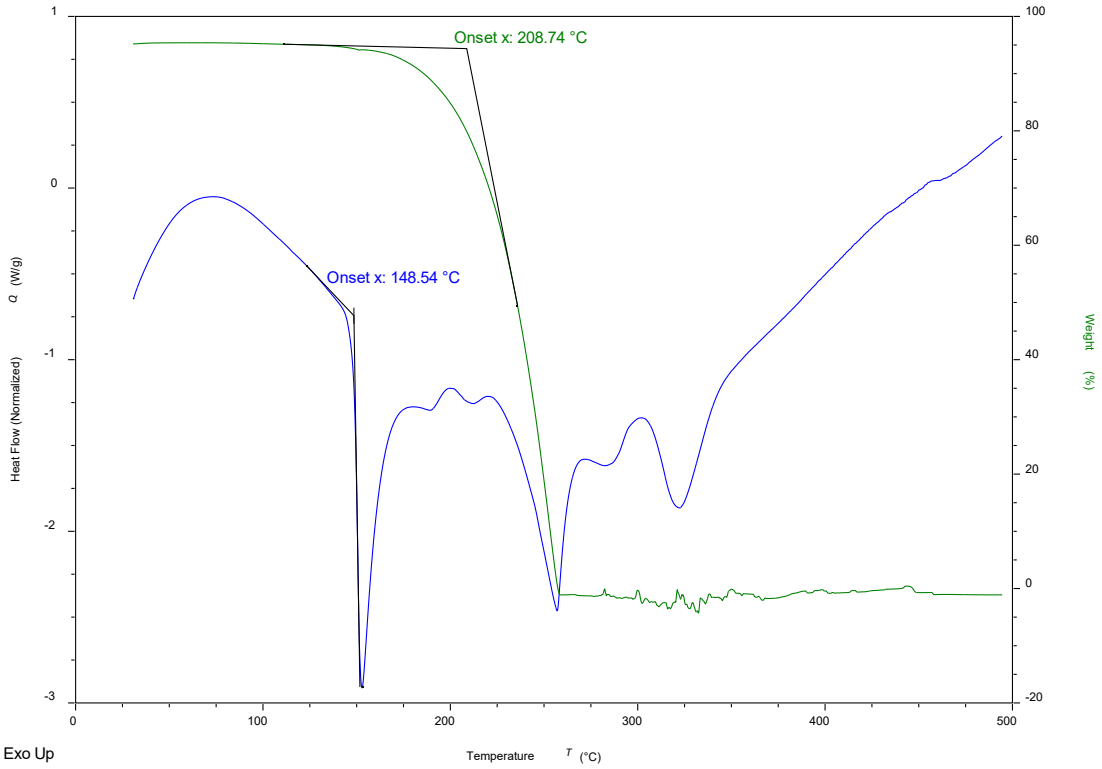

Figure SI16. SDT of (I_2F_8bph)(2,2'-bipy)

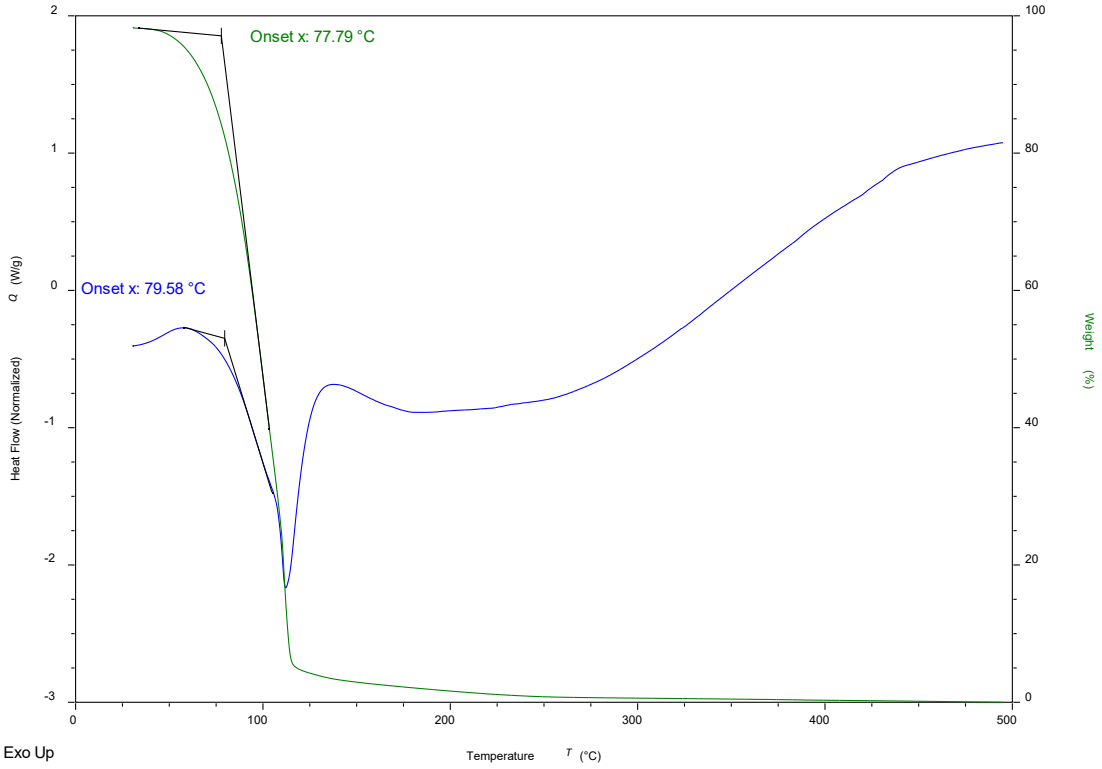

Figure SI17. SDT of (Br_2F_4bz)(4,4'-Me_2-2,2'-bipy)

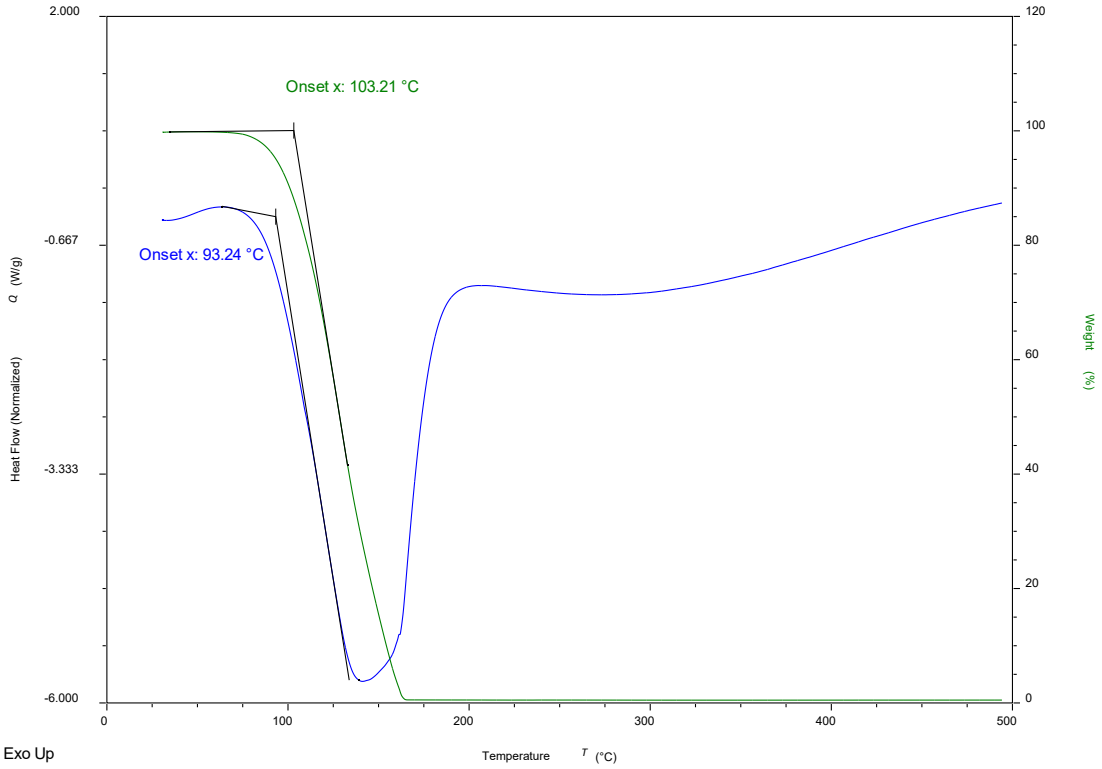

Figure SI18. SDT of (I_2F_4bz)(4,4'-Me_2-2,2'-bipy)

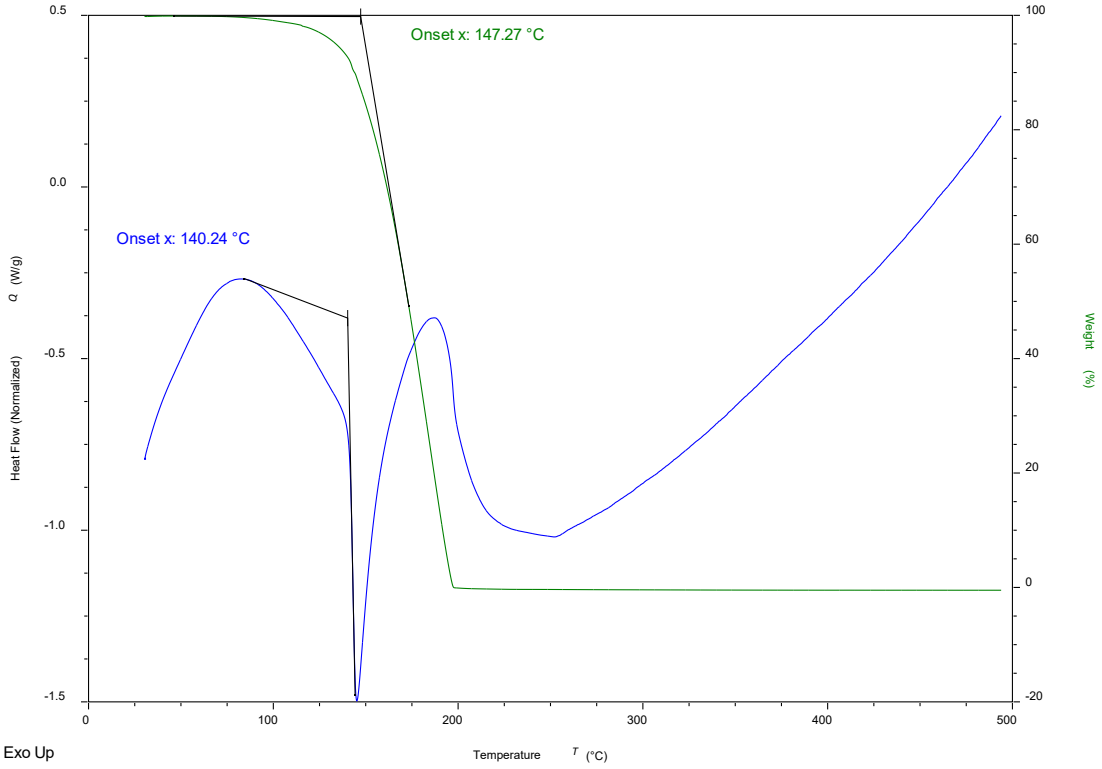

Figure SI19. SDT of (Br_2F_8bph)(4,4'-Me_2-2,2'-bipy)

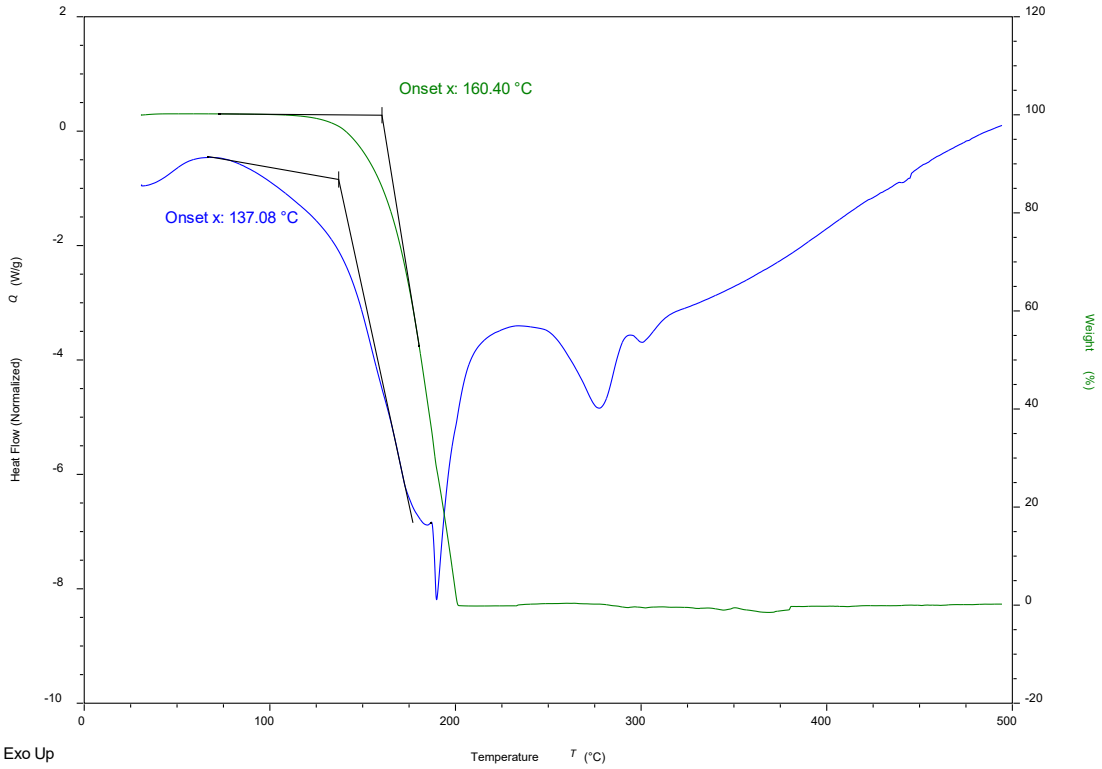

Figure SI20. SDT of (I_2F_8bph)(4,4'-Me_2-2,2'-bipy)

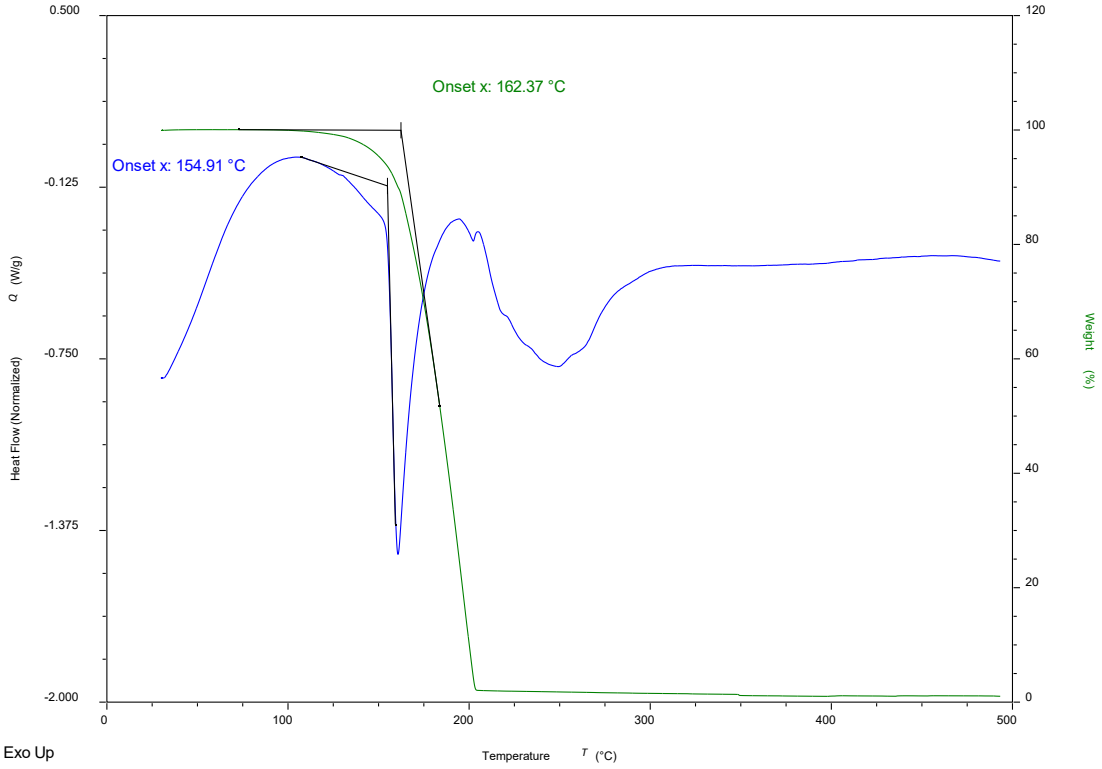

Figure SI21. SDT of (Br_2F_8bph)(4,4'-bipy)

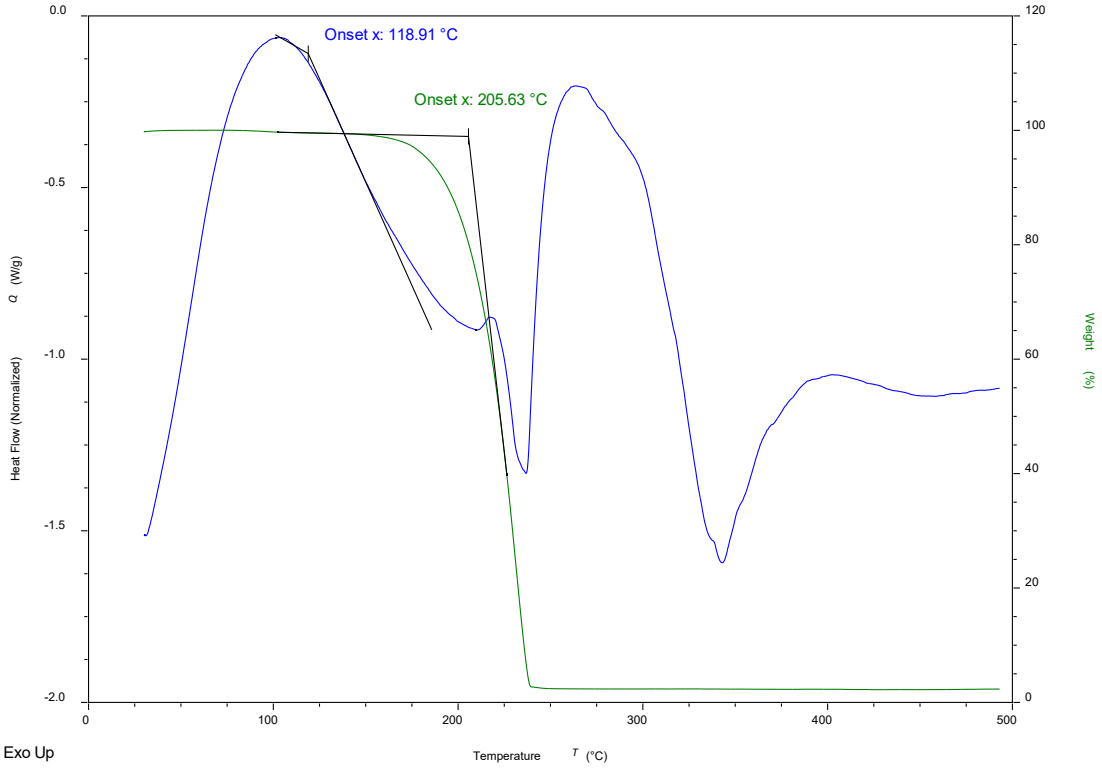

Figure SI22. SDT of (I_2F_8bph)(4,4'-bipy)

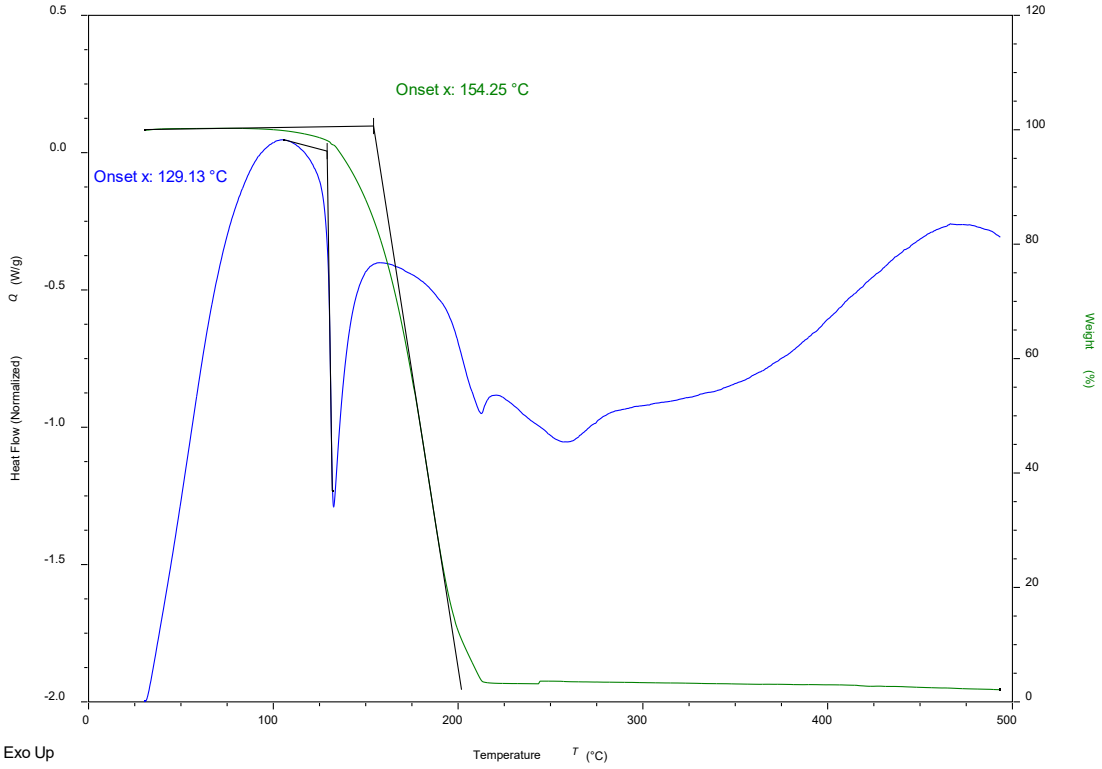

Figure SI23. SDT of $(Br_2F_8bph)(dpe)$

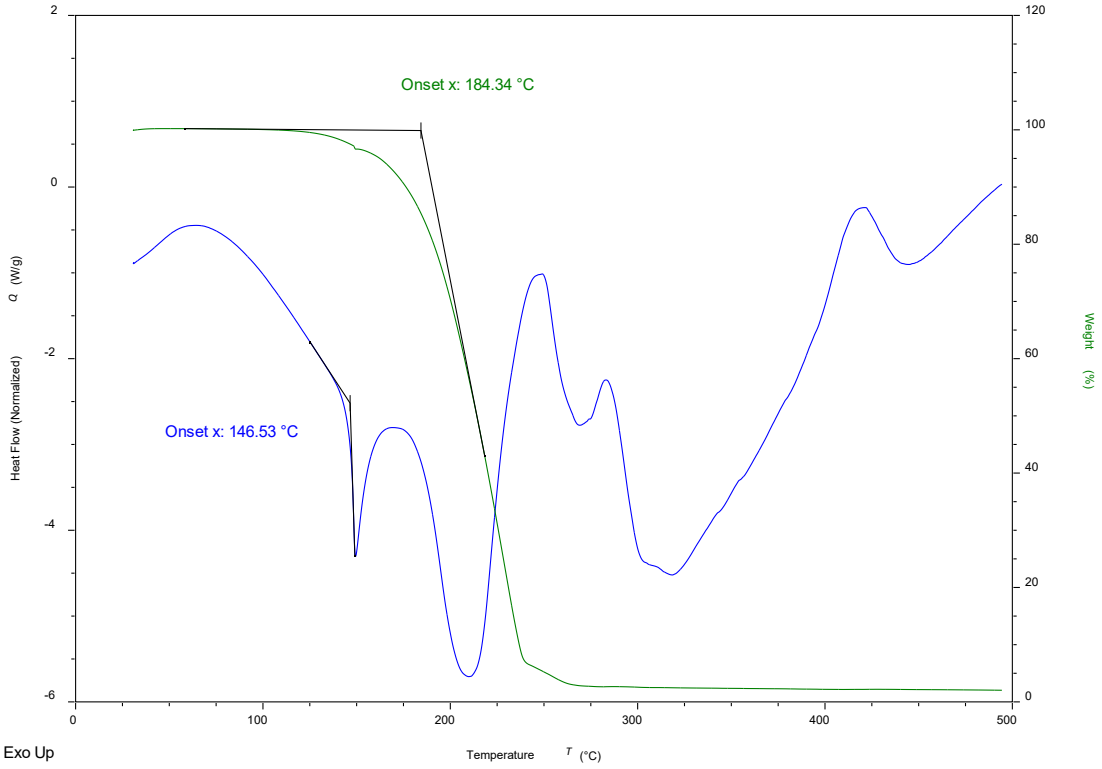

Figure SI24. SDT of $(Br_2F_8bph)_2(dpe)$

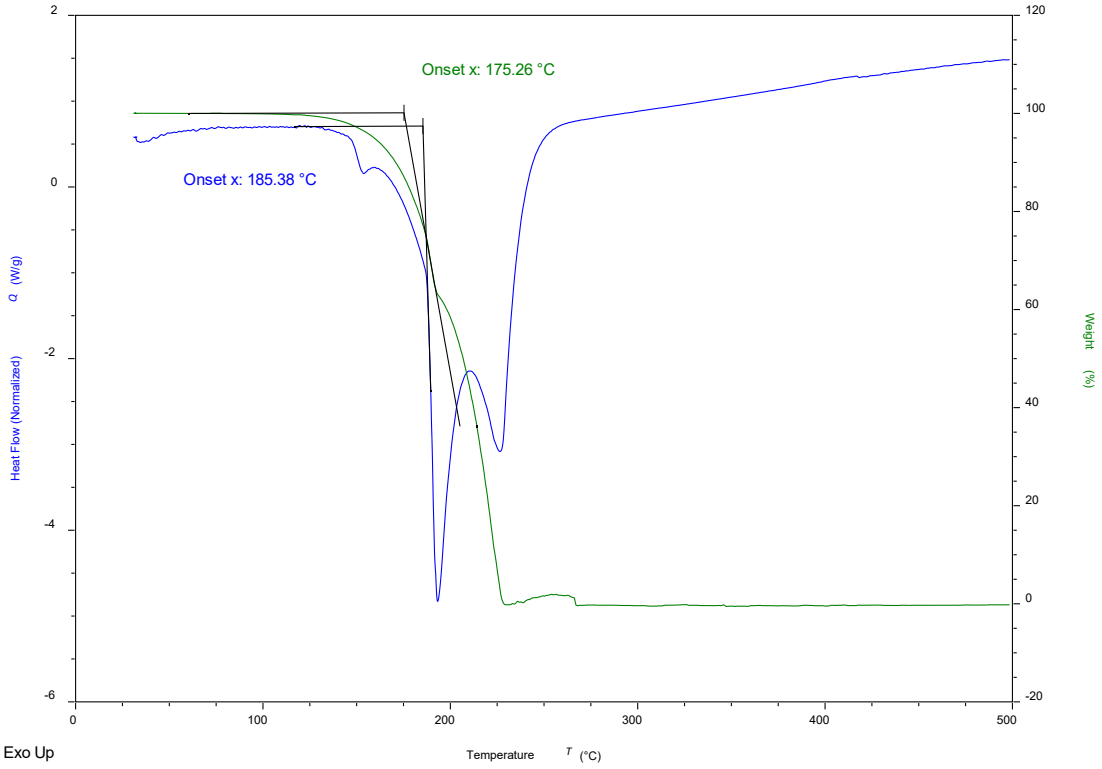

Figure SI25. SDT of (I_2F_8bph)(dpe)

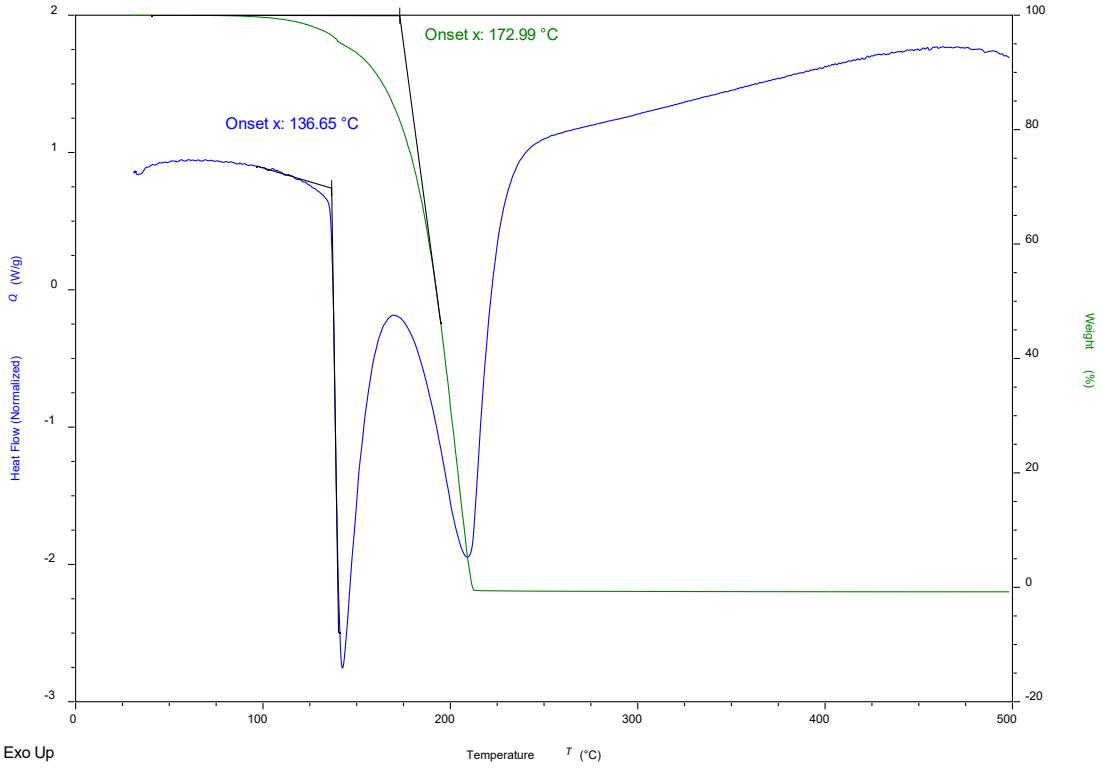

Figure SI26. SDT of (Br_2F_8bph)(DABCO)

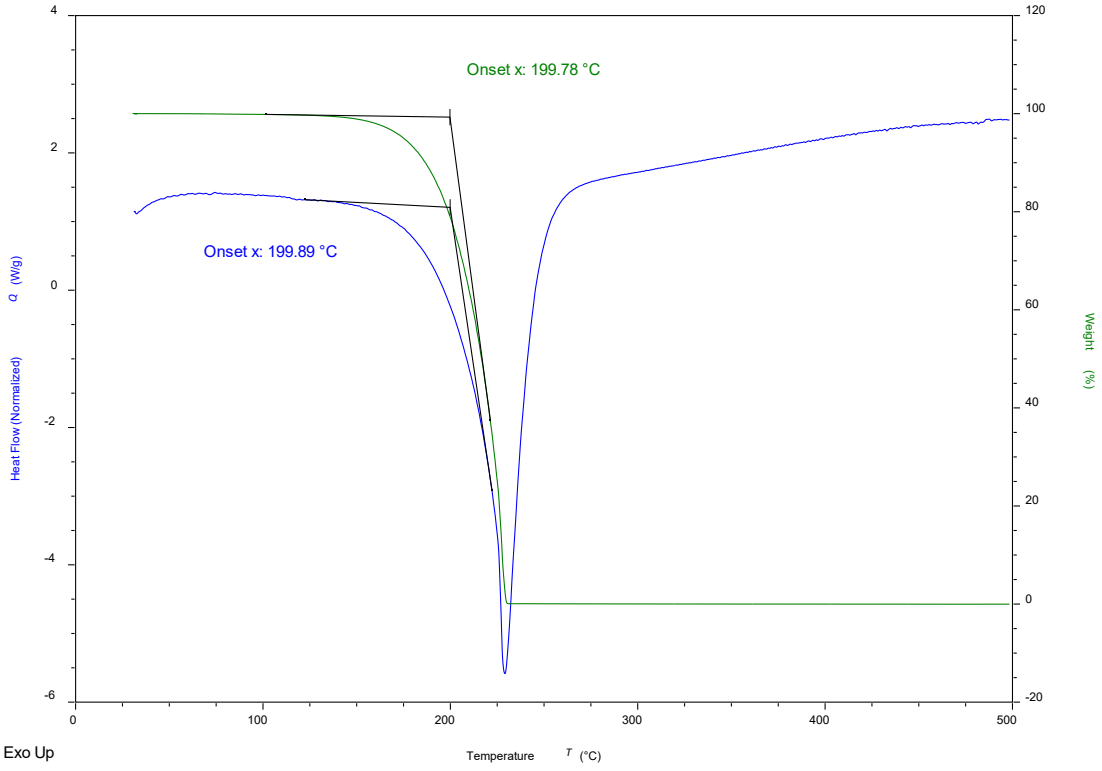

Figure SI27. SDT of (I_2F_8bph)(DABCO)

Table SI1. Crystallographic data and selected data collection parameters

Cocrystal	Br_2F_8bph	(Br_2F_4bz) (Me_2pyrz)	(I_2F_4bz) (Me_2pyrz)	(Br_2F_8bph) (Me_2pyrz)	(I_2F_8bph) (Me_2pyrz)	(I_2F_4bz) (Me_3pyrz)	(Br_2F_4bz) $(Me_4pyrz)_2$
Empirical formula	$Br_2C_{12}F_8$	$C_{12}H_8Br_2F_4N_2$	$C_{12}H_8F_4I_2N_2$	$C_{18}H_8Br_2F_8N_2$	$C_{18}H_8F_8I_2N_2$	$C_{13}H_{10}F_4I_2N_2$	$C_{22}H_{24}Br_2F_4N_4$
Formula weight (g/mol)	455.928	416.011	510.013	564.08	658.074	524.040	580.263
Crystal system	monoclinic	triclinic	triclinic	orthorhombic	orthorhombic	triclinic	monoclinic
Space group	$P2_1/n$	P-1	P-1	$Pna2_1$	$Pna2_1$	P-1	$P2_1/n$
T (K)	100.0	106(8)	106(8)	100.01	100.0	106(8)	100.0
a (Å)	13.2078(10)	4.8003(2)	5.7357(1)	12.9213(6)	12.6612(11)	7.7759(2)	7.0459(3)
b (Å)	7.3883(5)	6.6036(2)	6.2412(1)	12.3927(6)	12.5742(12)	9.1295(2)	14.8959(6)
c (Å)	13.6241(9)	10.9521(4)	10.6257(1)	11.7294(5)	12.2189(11)	11.6480(1)	11.1802(5)
α (°)	90	83.796(3)	86.110(1)	90	90	97.062(1)	90
β (°)	110.544(3)	84.121(3)	74.656(1)	90	90	95.417(1)	102.7101(15)
γ (°)	90	79.072(3)	77.418(1)	90	90	110.587(2)	90
V (Å^3)	1244.93(15)	337.69(2)	357.986(9)	1878.23(15)	1945.3(3)	759.74(3)	1144.66(9)
ρ_{calcd} (g·cm^{-3})	2.433	2.046	2.366	1.995	2.247	2.291	1.684
reflns collected	23306	23811	23215	14714	64662	53237	13976
Independent reflns	2968	1770	1878	3824	5019	3146	2362
R(int)	0.0502	0.0872	0.0574	0.0348	0.0570	0.0794	0.0432
# parameters	199	92	92	273	274	193	149
R_1 [$I>2\sigma(I)$]	0.0222	0.0280	0.0173	0.0216	0.0265	0.0302	0.0277
wR_2 [$I>2\sigma(I)$]	0.0459	0.0614	0.0373	0.0447	0.0650	0.0809	0.0593
R_1 (all)	0.0289	0.0329	0.0210	0.0309	0.0274	0.0350	0.0366
wR_2 (all)	0.0490	0.0626	0.0418	0.0473	0.0658	0.1058	0.0658
GooF	1.056	1.043	1.099	1.007	1.049	1.258	1.057
Flack parameter	N/A	N/A	N/A	0.014(7)	0.361(17)	N/A	N/A
CCDC #	2092652	2092653	2092654	2092655	2092656	2092657	2092658

Table SI1 (cont.). Crystallographic data and selected data collection parameters

Cocrystal	(Br_2F_8bph) (Me_4pyrz)	(I_2F_8bph) (Me_4pyrz)	(Br_2F_4bz) (quinox)	(Br_2F_8bph) (quinox)	(I_2F_8bph) (quinox)	(Br_2F_8bph) (phenaz)	(I_2F_8bph) (phenaz)
Empirical formula	$C_{20}H_{12}Br_2F_8N_2$	$C_{20}H_{12}F_8I_2N_2$	$C_{14}H_6Br_2F_4N_2$	$C_{20}H_6Br_2F_8N_2$	$C_{20}H_6F_8I_2N_2$	$C_{24}H_8Br_2F_8N_2$	$C_{24}H_8F_8I_2N_2$
Formula weight (g/mol)	592.126	686.128	438.018	586.078	680.080	636.139	730.141
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	triclinic	triclinic
Space group	*C*2/*c*	*C*2/*c*	$P2_1/n$	$P2_1/c$	$P2_1/c$	*P*-1	*P*-1
T (K)	100.0	100.0	100.01	100.0	100.0	101.0	100.01
a (Å)	13.3837(9)	13.8570(6)	11.499(1)	8.0424(4)	8.2738(5)	7.6092(4)	7.7139(6)
b (Å)	13.8699(10)	13.7638(6)	6.2670(5)	7.0976(4)	6.9896(4)	12.2473(7)	12.2385(10)
c (Å)	11.1754(8)	11.5041(5)	19.9650(18)	33.8513(17)	34.5606(18)	12.8900(8)	13.5005(11)
α (°)	90	90	90	90	90	111.115(2)	113.307(3)
β (°)	102.784(3)	104.737(2)	98.291(3)	94.497(2)	93.006(2)	100.664(2)	99.272(3)
γ (°)	90	90	90	90	90	95.114(2)	94.932(3)
V (Å^3)	2023.1(3)	2121.94(16)	1423.7(2)	1926.34(17)	1995.9(2)	1085.22(11)	1139.37(16)
ρ_{calcd} (g·cm^{-3})	1.944	2.148	2.043	2.021	2.263	1.947	2.128
reflns collected	16444	13646	24244	15647	39071	37287	33909
Independent reflns	2309	2251	3557	3778	3924	4612	4656
R(int)	0.0268	0.0352	0.0397	0.0499	0.0418	0.0300	0.0307
# parameters	147	147	199	289	289	325	325
R_1 [$I>2\sigma(I)$]	0.0162	0.0164	0.0208	0.0341	0.0171	0.0182	0.0143
wR_2 [$I>2\sigma(I)$]	0.0412	0.0389	0.0463	0.0812	0.0361	0.0413	0.0340
R_1 (all)	0.0179	0.0186	0.0290	0.0521	0.0210	0.0222	0.0163
wR_2 (all)	0.0421	0.0410	0.0523	0.0928	0.0388	0.0437	0.0355
GooF	1.031	1.048	1.066	1.067	1.061	1.071	1.063
Flack parameter	N/A	N/A	N/A	N/A	N/A	N/A	N/A
CCDC #	2092659	2092660	2093037	2092661	2093039	2093038	2093040

Table SI1 (cont.). Crystallographic data and selected data collection parameters

Cocrystal	(Br_2F_4bz) (2,2'-bipy)	(Br_2F_8bph) (2,2'-bipy)	(I_2F_8bph) (2,2'-bipy)	(Br_2F_4bz) (Me_2-2,2'-bipy)	(I_2F_4bz) (Me_2-2,2'-bipy)	(Br_2F_8bph) (Me_2-2,2'-bipy)
Empirical formula	$C_{16}H_8Br_2F_4N_2$	$C_{44}H_{16}Br_4F_{16}N_4$	$C_{22}H_8F_8I_2N_2$	$C_{18}H_{12}Br_2F_4N_2$	$C_{18}H_{12}F_4I_2N_2$	$C_{24}H_{12}Br_2F_8N_2$
Formula weight (g/mol)	464.056	1224.25	706.118	492.110	586.112	640.170
Crystal system	triclinic	monoclinic	monoclinic	triclinic	orthorhombic	triclinic
Space group	*P*-1	$P2_1/c$	$P2_1/c$	*P*-1	*Aea*2	*P*-1
T (K)	99.99	100.01	100.0	100.0	100.0	100.01
a (Å)	6.8925(9)	7.6382(4)	7.7281(2)	6.8796(6)	13.1529(17)	7.7760(4)
b (Å)	7.6625(10)	15.0660(8)	7.6981(3)	7.4209(6)	18.502(3)	10.0737(6)
c (Å)	8.6230(12)	35.9783(18)	36.2272(13)	9.2086(8)	15.239(3)	14.8950(9)
α (°)	108.019(5)	90	90	82.848(3)	90	81.781(2)
β (°)	97.023(5)	90.815(2)	91.551(1)	82.965(3)	90	78.260(2)
γ (°)	109.558(4)	90	90	75.554(3)	90	83.082(2)
V (Å^3)	394.92(9)	4139.9(4)	2154.43(13)	449.67(7)	3708.5(9)	1125.59(11)
ρ_{calcd} (g·cm^{-3})	1.951	1.964	2.177	1.817	2.100	1.889
reflns collected	9852	67217	15906	10929	33906	74967
Independent reflns	1966	8794	4889	2068	4596	6318
R(int)	0.0314	0.0520	0.0341	0.0305	0.0520	0.0413
# parameters	109	613	307	119	237	327
R_1 [$I>2\sigma(I)$]	0.0199	0.0265	0.0249	0.0258	0.0239	0.0193
wR_2 [$I>2\sigma(I)$]	0.0425	0.0544	0.0495	0.0682	0.0447	0.0468
R_1 (all)	0.0236	0.0377	0.0299	0.0294	0.0316	0.0235
wR_2 (all)	0.0455	0.0593	0.0518	0.0720	0.0503	0.0491
GooF	1.072	1.074	1.066	1.054	1.061	1.053
Flack parameter	N/A	N/A	N/A	N/A	-0.03(3)	N/A
CCDC #	2093041	2093042	2093043	2093044	2093045	2093046

Table SI1 (cont.). Crystallographic data and selected data collection parameters

Cocrystal	(I_2F_8bph) (Me_2-2,2'-bipy)	(Br_2F_8bph) (4,4'-bipy)	(I_2F_8bph) (4,4'-bipy)	(Br_2F_8bph) (dpe)	(Br_2F_8bph)$_2$ (dpe)	(I_2F_8bph) (dpe)
Empirical formula	$C_{24}H_{12}F_8I_2N_2$	$C_{22}H_8Br_2F_8N_2$	$C_{22}H_8F_8I_2N_2$	$C_{24}H_{10}Br_2F_8N_2$	$C_{36}H_{10}Br_4F_{16}N_2$	$C_{24}H_{10}F_8I_2N_2$
Formula weight (g/mol)	734.172	612.116	706.118	638.155	1094.082	732.156
Crystal system	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic
Space group	*P*-1	*P*-1	*P*-1	*P*-1	*P*-1	*P*-1
T (K)	100.0	150.15	100.0	100.01	100.0	100.0
a (Å)	7.9933(7)	7.7409(4)	7.9217(5)	7.3598(5)	7.4148(5)	7.9651(5)
b (Å)	10.050(1)	11.2944(6)	11.1526(9)	11.2484(8)	11.4097(7)	10.8942(7)
c (Å)	15.0745(14)	12.7419(8)	12.8382(10)	13.8819(10)	21.1980(12)	14.4024(10)
α (°)	80.124(3)	73.313(2)	105.190(4)	88.308(3)	90.035(2)	108.756(2)
β (°)	78.660(3)	72.443(2)	107.580(2)	78.403(2)	90.010(2)	105.483(2)
γ (°)	83.953(3)	89.944(2)	90.334(3)	76.782(2)	107.163(2)	90.273(3)
V (Å^3)	1166.52(19)	1012.9(1)	1039.01(14)	1095.78(13)	1713.50(18)	1134.80(13)
ρ_{calcd} (g·cm^{-3})	2.090	2.007	2.257	1.934	2.121	2.143
reflns collected	49406	22875	61424	18362	21406	36775
Independent reflns	5563	3973	4423	4267	7010	4686
R(int)	0.0389	0.1433	0.0621	0.0343	0.0357	0.0409
# parameters	327	307	307	325	523	325
R_1 [$I>2\sigma(I)$]	0.0168	0.0554	0.0453	0.0288	0.0243	0.0236
wR_2 [$I>2\sigma(I)$]	0.0389	0.1159	0.0884	0.0586	0.0529	0.0503
R_1 (all)	0.0184	0.0785	0.0613	0.0359	0.0319	0.0308
wR_2 (all)	0.0397	0.1231	0.0951	0.0605	0.0565	0.0580
GooF	1.061	1.049	1.065	1.077	1.057	1.090
Flack parameter	N/A	N/A	N/A	N/A	N/A	N/A
CCDC #	2092666	2092665	2092667	2092668	2092669	2092670

Table SI1 (cont.). Crystallographic data and selected data collection parameters

Cocrystal	(Br_2F_8bph) (DABCO)	(Br_2F_8bph)$_2$ (DABCO)	(I_2F_8bph) (DABCO)
Empirical formula	$C_{18}H_{12}Br_2F_8N_2$	$C_{45}H_{18}Br_6F_{24}N_3$	$C_{18}H_{12}F_8I_2N_2$
Formula weight (g/mol)	568.104	1536.047	662.105
Crystal system	monoclinic	triclinic	monoclinic
Space group	$P2_1/n$	P-1	$P2_1/n$
T (K)	100.01	100.0	100.0
a (Å)	13.1047(10)	7.938(3)	13.5292(11)
b (Å)	10.8097(8)	10.577(4)	10.9229(8)
c (Å)	14.1460(11)	29.826(11)	14.122(1)
α (°)	90	91.873(11)	90
β (°)	107.369(3)	94.086(13)	108.470(3)
γ (°)	90	105.304(11)	90
V (Å^3)	1912.5(3)	2405.8(15)	1979.4(3)
ρ_{calcd} (g·cm^{-3})	1.973	2.120	2.222
reflns collected	27928	69289	32240
Independent reflns	3921	11063	4711
R(int)	0.0592	0.0537	0.0290
# parameters	271	739	271
R_1 [$I>2\sigma(I)$]	0.0297	0.0285	0.0191
wR_2 [$I>2\sigma(I)$]	0.0594	0.0550	0.0436
R_1 (all)	0.0449	0.0410	0.0223
wR_2 (all)	0.0661	0.0620	0.0470
GooF	1.028	1.069	1.054
Flack parameter	N/A	N/A	N/A
CCDC #	2092671	2092672	2092673

Table SI2. Halogen bond parameters

Cocrystal		$D_{X\cdots N}$	R_{XB}[a]	$\theta_{C-X\cdots N}$	Ph-Ph θ[b]	$\theta_{I\cdots N\cdots Y}$	REFCODE
(Br_2F_4bz)(Me_2pyrz)	Br1···N1	2.889(2)	0.85	177.23(8)	–	162.71(12)	
(I_2F_4bz)(Me_2pyrz)	I1···N1	2.897(2)	0.82	178.11(7)	–	167.05(12)	
(Br_2F_8bph)(Me_2pyrz)	Br1···N1	2.897(2)	0.85	177.85(10)	53.94(8)	178.94(10)	
	Br2···N2	2.929(3)	0.86	179.2(1)		175.75(11)	
(I_2F_8bph)(Me_2pyrz)	I1···N1	2.882(4)	0.82	173.90(13)	55.09(12)	171.5(2)	
	I2···N2	2.881(4)	0.82	176.74(13)		174.31(18)	
(I_2F_4bz)(Me_3pyrz)	I1···N1	2.909(4)	0.82	178.51(16)	–	171.37(19)	
	I2···N2	3.007(4)	0.85	175.37(16)	–	177.53(15)	
(Br_2F_4bz)(Me_4pyrz)$_2$	Br1···N1	2.899(2)	0.85	170.73(10)	–	161.65(13)	
(I_2F_4bz)(Me_4pyrz)	I1···N1	3.0665(18)	0.87	177.15(8)	–	178.01(12)	JAQMAQ[1]
(Br_2F_8bph)(Me_4pyrz)	Br1···N1	2.9961(12)	0.88	172.76(5)	52.44(7)	175.59(7)	
(I_2F_8bph)(Me_4pyrz)	I1···N1	3.0187(19)	0.86	174.57(7)	52.72(10)	174.33(11)	
(Br_2F_4bz)(quinox)	Br1···N1	2.9333(16)	0.86	172.84(7)	–	157.05(7)	
	Br2···N2	2.9296(16)	0.86	171.64(7)	–	160.39(7)	
(I_2F_4bz)(quinox)	I1···N1	2.954(3)	0.84	172.15(12)	–	156.40(16)	WIGVAM[2]
	I2···N2	2.959(4)	0.84	173.05(13)	–	161.10(17)	
(Br_2F_8bph)(quinox)	Br1···N1	2.883(3)	0.85	171.96(13)	53.77(13)	161.24(14)	
	Br2···N2	2.901(3)	0.85	173.77(13)		156.17(14)	
(I_2F_8bph)(quinox)	I1···N1	2.893(2)	0.82	173.01(8)	54.79(8)	161.80(9)	
	I2···N2	2.917(2)	0.83	173.60(8)		158.18(9)	
(Br_2F_4bz)(phenaz)	Br1···N2	2.985(2)	0.88	172.59(8)	–	171.33(9)	VOMGUA[3]
(I_2F_4bz)(phenaz)	I1···N1	2.970(3)	0.84	175.45(11)	–	170.08(14)	VOMHAH[3]
(Br_2F_8bph)(phenaz)	Br1···N1	2.8789(14)	0.85	174.95(6)	53.48(6)	153.40(9)	
	Br2···N2	2.9957(14)	0.88	177.47(6)		167.75(8)	
(I_2F_8bph)(phenaz)	I1···N1	2.9132(16)	0.83	176.17(6)	53.73(7)	156.77(10)	
	I2···N2	2.9955(16)	0.85	176.10(6)		172.70(9)	
(Br_2F_4bz)(2,2'-bipy)	Br1···N1	3.0802(16)	0.91	169.16(6)	–	154.01(7)	
(I_2F_4bz)(2,2'-bipy)	I1···N1	3.158(3)	0.89	169.61(13)	–	145.29(13)	ISIJEZ01[1]
(Br_2F_8bph)(2,2'-bipy)	Br1···N1	2.996(2)	0.88	165.58(8)	54.17(8)	152.86(9)	
	Br2···N2	3.107(2)	0.91	160.95(8)		153.93(9)	
	Br3···N3	2.929(2)	0.86	167.03(9)	54.24(8)	150.63(10)	
	Br4···N4	3.068(2)	0.90	165.50(8)		151.95(9)	
(I_2F_8bph)(2,2'-bipy)	I1···N1	3.058(2)	0.86	168.16(9)	53.36(10)	155.11(11)	
	I2···N2	3.091(2)	0.88	164.23(9)		153.53(11)	
(Br_2F_4bz)(Me_2-2,2'-bipy)	Br1···N1	3.012(2)	0.89	175.77(10)	–	157.42(11)	
(I_2F_4bz)(Me_2-2,2'-bipy)	I1···N1	3.021(4)	0.86	173.79(15)	–	157.26(19)	

	I2···N2	3.068(4)	0.87	170.05(13)	–	157.90(17)	
(Br_2F_8bph)(Me_2-2,2'-bipy)	Br1···N1	2.8964(11)	0.85	169.28(5)	58.60(4)	154.86(5)	
	Br2···N2	3.0034(12)	0.88	161.43(5)		156.79(5)	
(I_2F_8bph)(Me_2-2,2'-bipy)	I1···N1	2.9248(15)	0.83	169.09(6)	59.47(6)	156.99(7)	
	I2···N2	3.0508(15)	0.86	162.35(6)		157.90(7)	
(Br_2F_4bz)(4,4'-bipy)	Br1A···N4C	2.8778(13)	0.85	177.21(4)	–	162.20(5)	IKUJUT[4]
	Br1B···N4D	2.9791(12)	0.88	176.40(4)	–	155.93(5)	
(I_2F_4bz)(4,4'-bipy)	I1···N1	2.8218(13)	0.80	177.13(5)	–	162.56(7)	QIHBEO02[5]
(Br_2F_8bph)(4,4'-bipy)	Br1···N1	2.749(6)	0.81	179.1(2)	61.0(2)	177.6(3)	
	Br2···N2	2.789(6)	0.82	178.4(2)		179.3(3)	
(I_2F_8bph)(4,4'-bipy)	I1···N1	2.734(6)	0.77	179.5(2)	61.6(2)	178.6(3)	
	I2···N2	2.752(6)	0.78	178.3(2)		179.2(3)	
(Br_2F_4bz)(dpe)	Br···N5	2.8293(13)	0.83	179.07(5)	–	175.43(6)	IKUHUR03[6]
(I_2F_4bz)(dpe)	I···N	2.7677(14)	0.78	179.28(5)	–	177.15(5)	QIHCAL06[6]
(Br_2F_8bph)(dpe)	Br1···N1	2.873(3)	0.85	169.7(1)	57.52(10)	156.95(11)	
	Br2···N2	2.909(3)	0.86	167.82(10)		166.54(12)	
(Br_2F_8bph)$_2$(dpe)	Br1···N1	2.888(2)	0.85	169.13(8)	58.30(7)	164.94(10)	
	Br3···N2	2.899(2)	0.85	166.45(9)	55.41(7)	158.79(10)	
(I_2F_8bph)(dpe)	I1···N1	2.736(3)	0.77	177.32(11)	62.35(11)	173.74(14)	
	I2···N2	2.711(3)	0.77	178.08(11)		173.01(14)	
(Br_2F_4bz)(DABCO)	Br27···N7	2.9101(18)	0.86	169.57(10)	–	159.83(12)	DIVDUI[7]
	Br28···N8	2.8936(17)	0.85	167.69(10)	–	162.31(12)	
(I_2F_4bz)(DABCO)	I1···N1	2.7350(8)	0.77	173.24(3)	–	173.63(4)	ISIHUN03[8]
	I2···N2	2.7438(8)	0.78	173.94(3)	–	172.49(4)	
(Br_2F_8bph)(DABCO)	Br1···N1	2.693(2)	0.79	176.37(10)	56.14(10)	177.13(12)	
	Br2···N2	2.703(2)	0.80	175.54(10)		177.46(12)	
(Br_2F_8bph)$_2$(DABCO)	Br1···N1	2.780(2)	0.82	169.84(11)	55.95(10)	164.45(10)	
	Br3···N2	2.823(2)	0.83	170.01(11)	59.54(11)	165.11(10)	
	Br5···N3	2.670(18)	0.79	174.6(4)	52.32(10)	177.6(8)	
	Br5···N4	2.674(18)	0.79	178.9(3)		174.2(8)	
(I_2F_8bph)(DABCO)	I1···N1	2.6652(19)	0.76	177.26(7)	54.05(8)	178.12(10)	
	I2···N2	2.6830(19)	0.76	176.35(7)		178.63(9)	

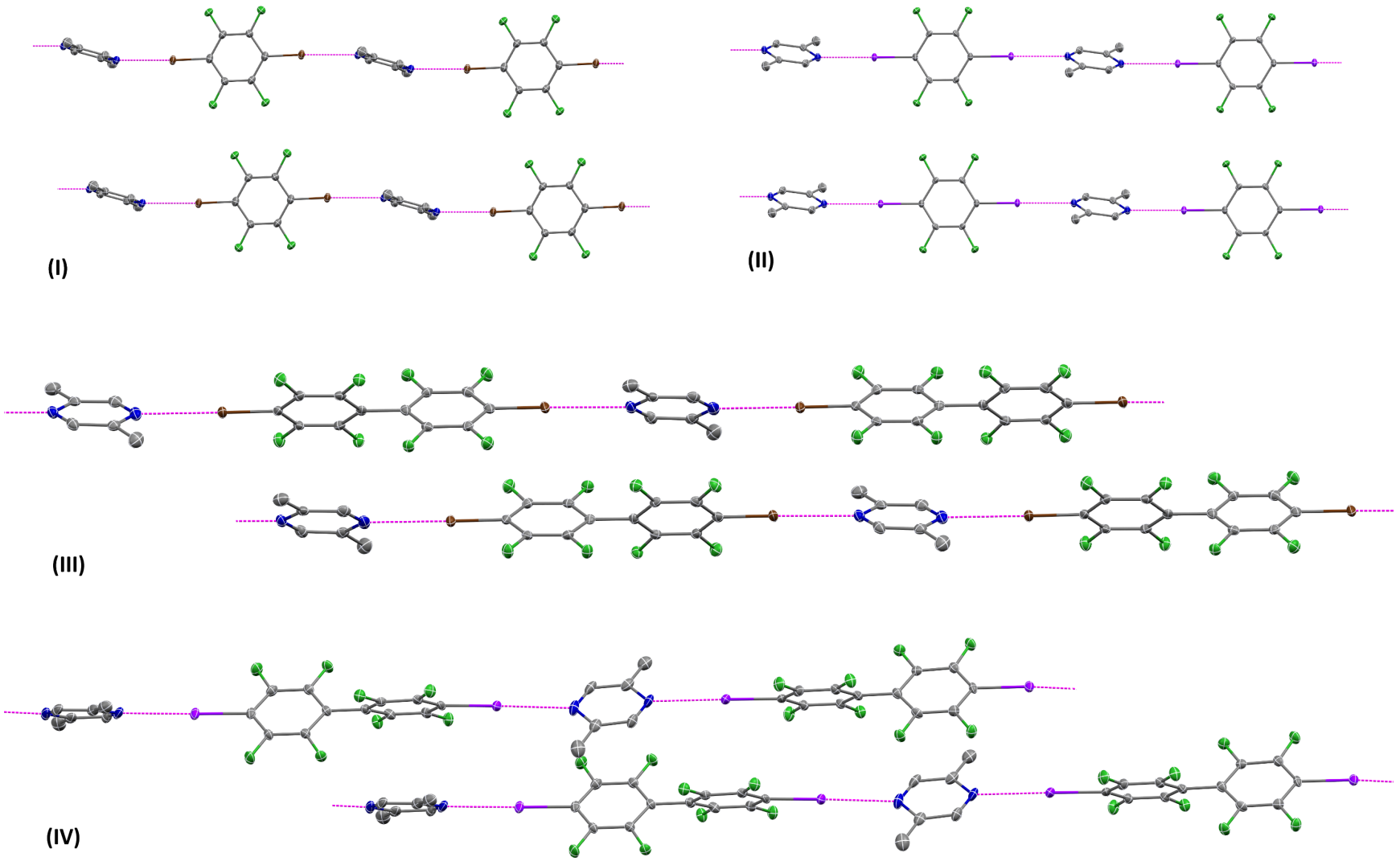

Figure SI28. Neighboring 1-d halogen bonding chains in (Br_2F_4bz)(Me_2pyrz) (I), (I_2F_4bz)(Me_2pyrz) (II), (Br_2F_8bph)(Me_2pyrz) (III), and (I_2F_8bph)(Me_2pyrz) (IV). Halogen bonds are shown as magenta dashed lines.

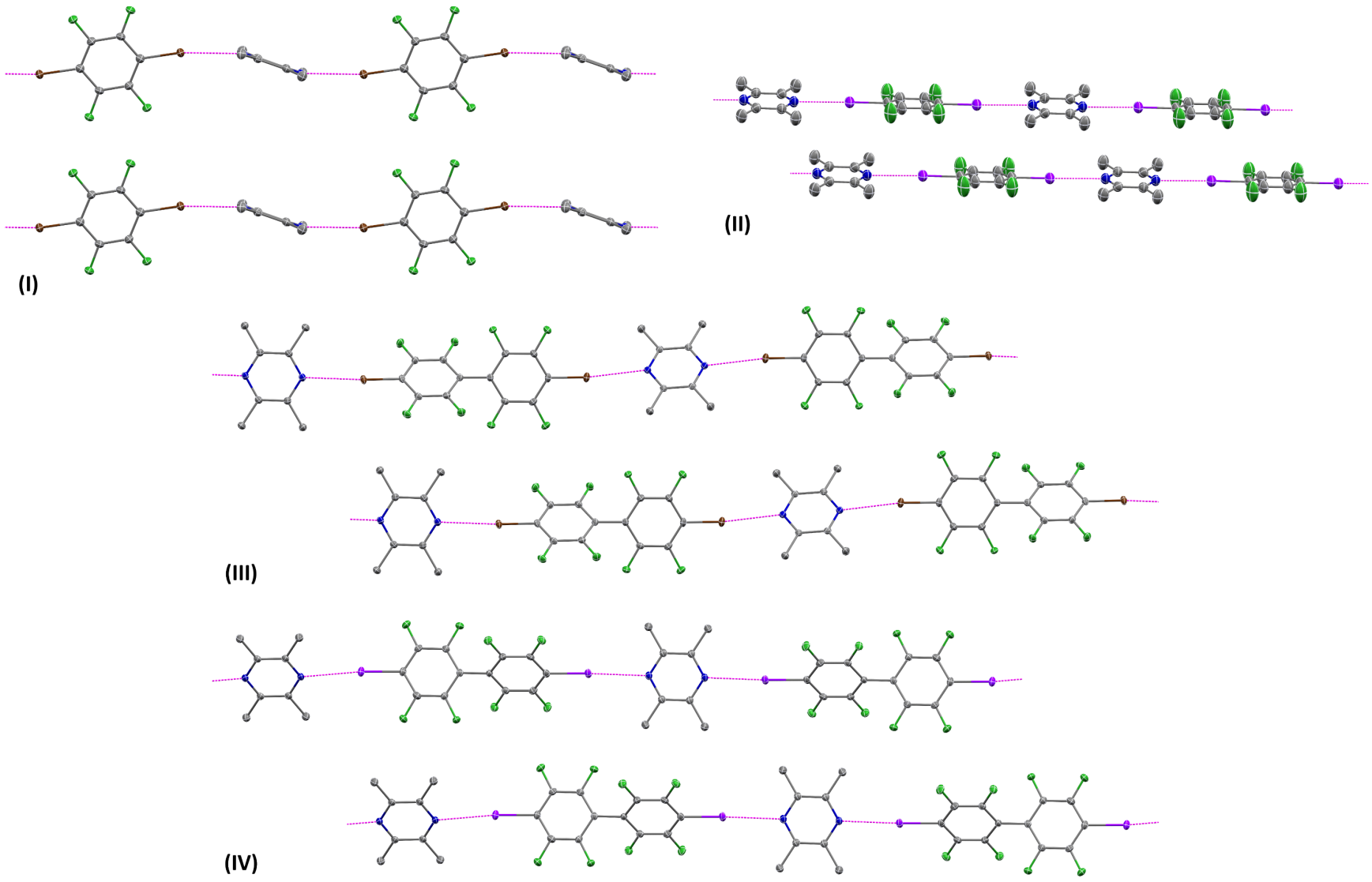

Figure SI29. Neighboring 1-d halogen bonding chains in $(Br_2F_4bz)_2(Me_4pyrz)$ (I), $(I_2F_4bz)(Me_4pyrz)$ (II), $(Br_2F_8bph)(Me_4pyrz)$ (III), and $(I_2F_8bph)(Me_4pyrz)$ (IV). Halogen bonds are shown as magenta dashed lines.

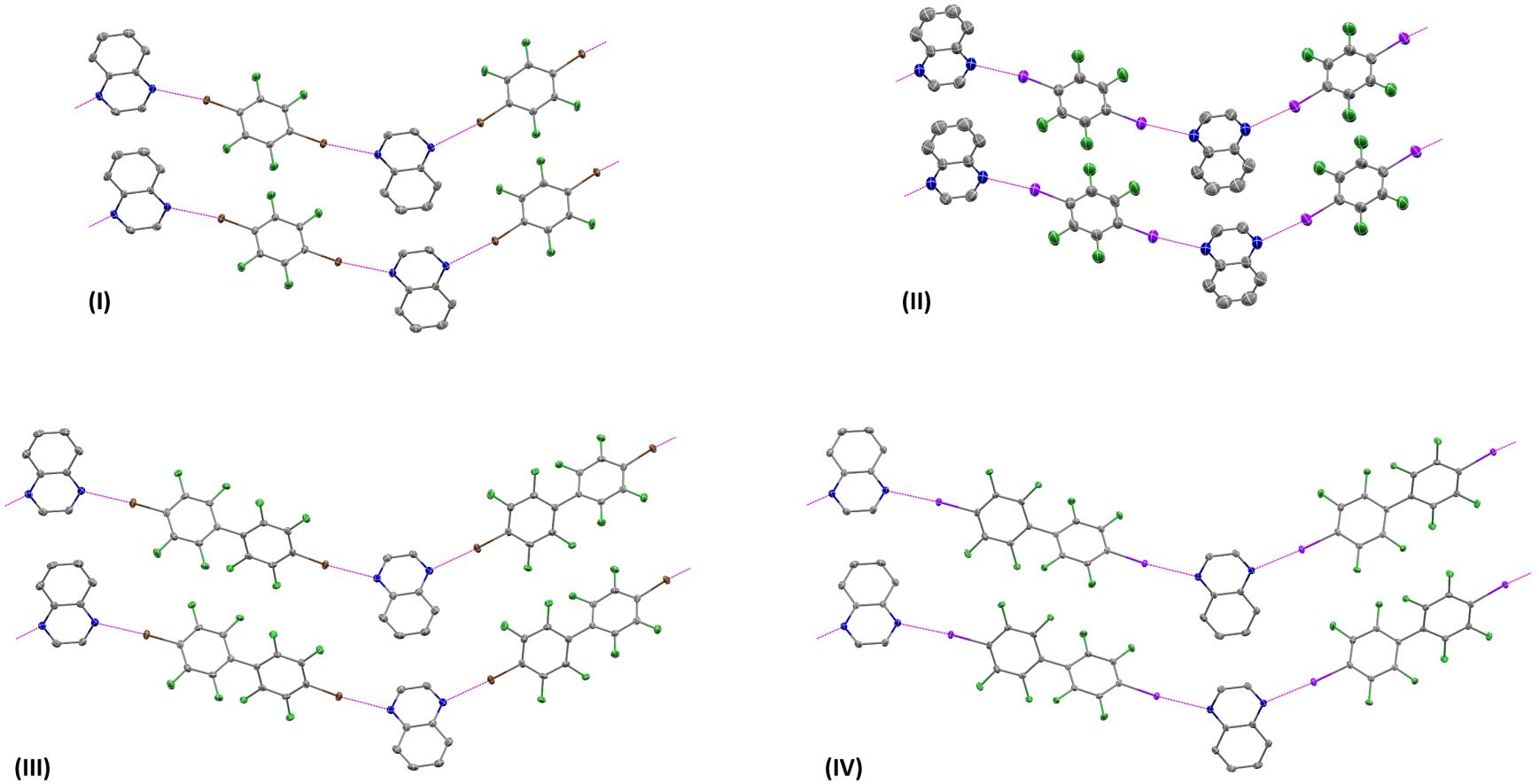

Figure SI30. Neighboring 1-d halogen bonding chains in (Br_2F_4bz)(quinox) (I), (I_2F_4bz)(quinox) (II), (Br_2F_8bph)(quinox) (III), and (I_2F_8bph)(quinox) (IV). Halogen bonds are shown as magenta dashed lines.

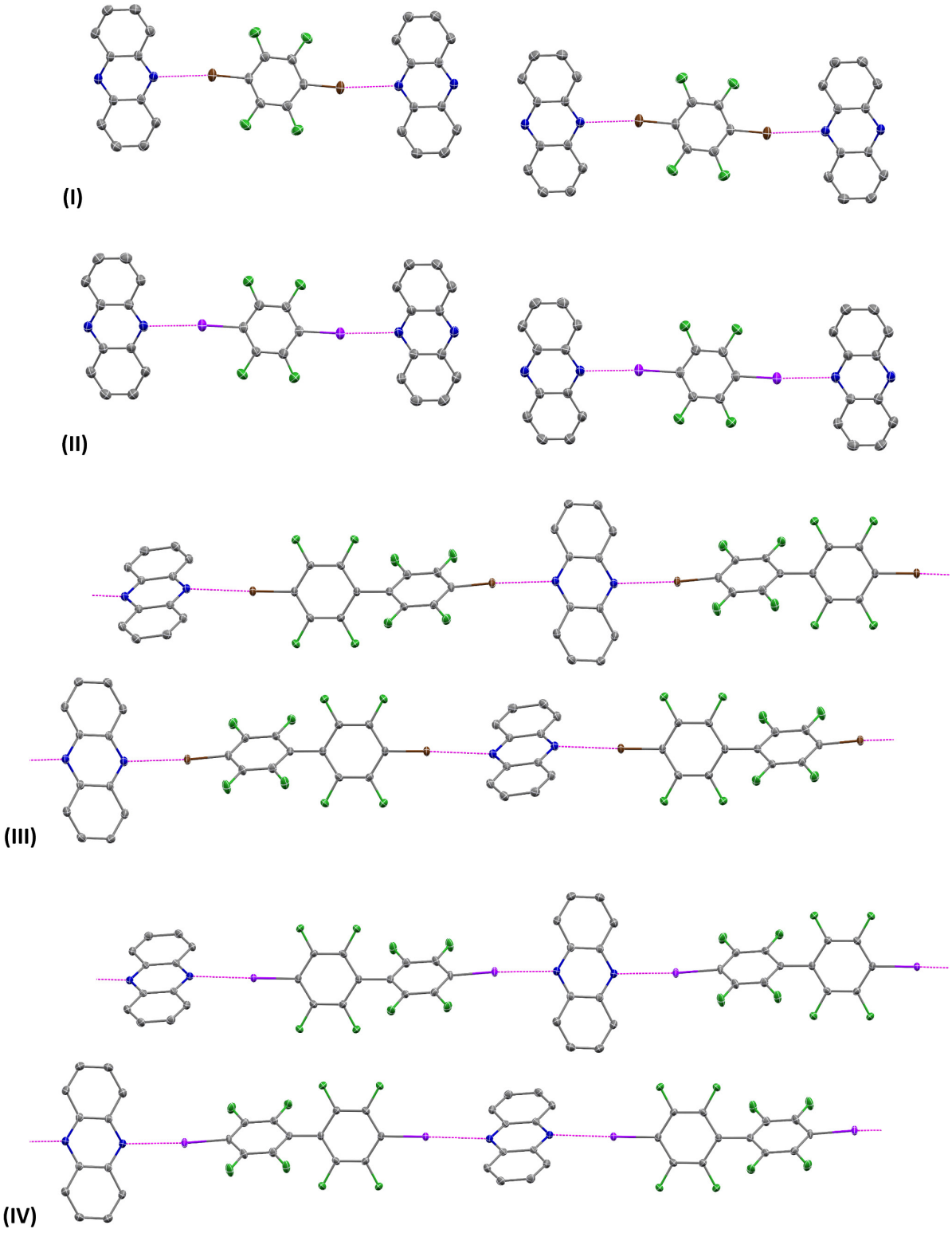

Figure SI31. Neighboring 1-d halogen bonding chains in (Br_2F_4bz)(phenaz) (I), (I_2F_4bz)(phenaz) (II), (Br_2F_8bph)(phenaz) (III), and (I_2F_8bph)(phenaz) (IV). Halogen bonds are shown as magenta dashed lines.

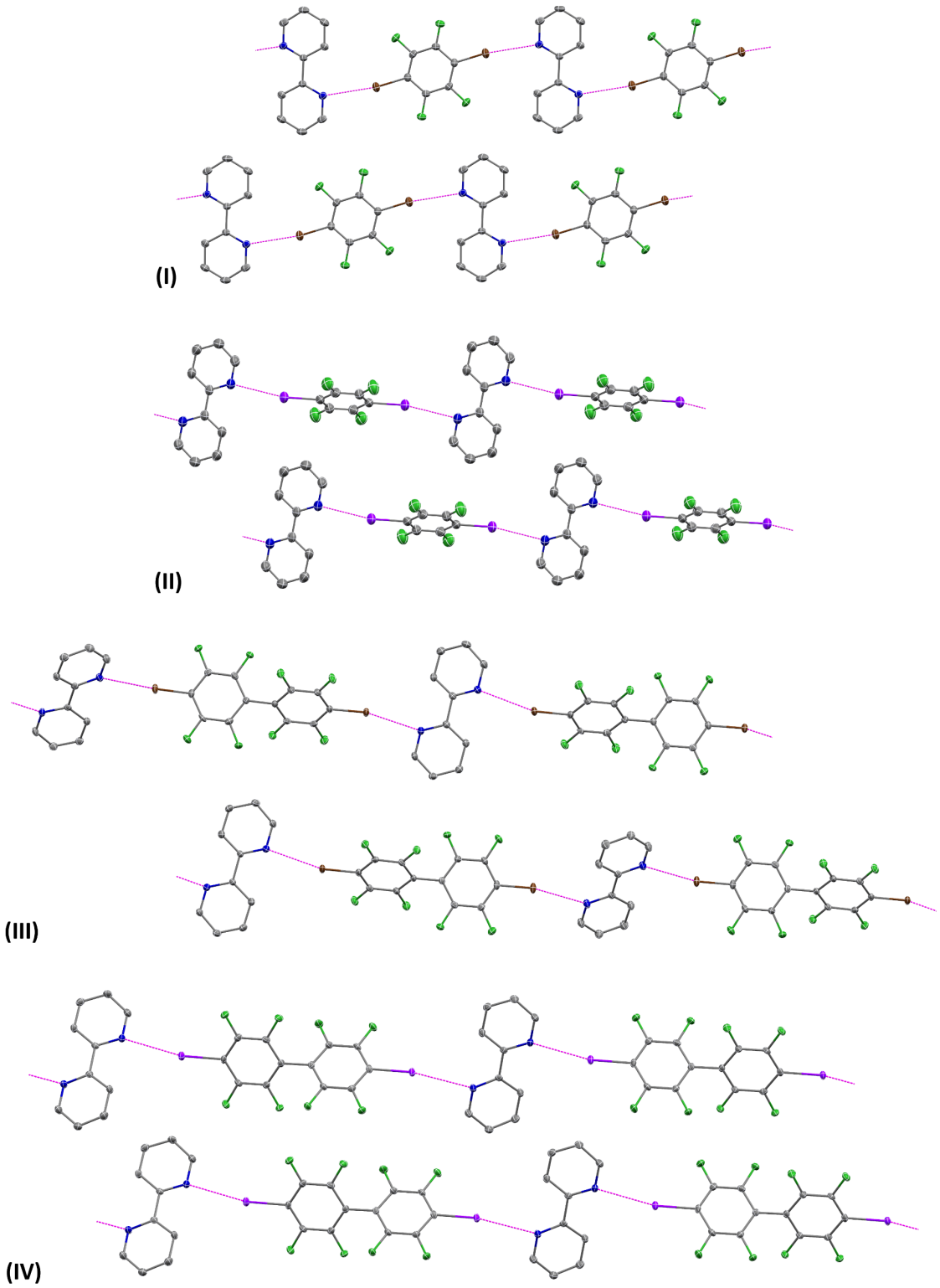

Figure SI32. Neighboring 1-d halogen bonding chains in (Br_2F_4bz)(2,2'-bipy) (I), (I_2F_4bz)(2,2'-bipy) (II), (Br_2F_8bph)(2,2'-bipy) (III), and (I_2F_8bph)(2,2'-bipy) (IV). Halogen bonds are shown as magenta dashed lines.

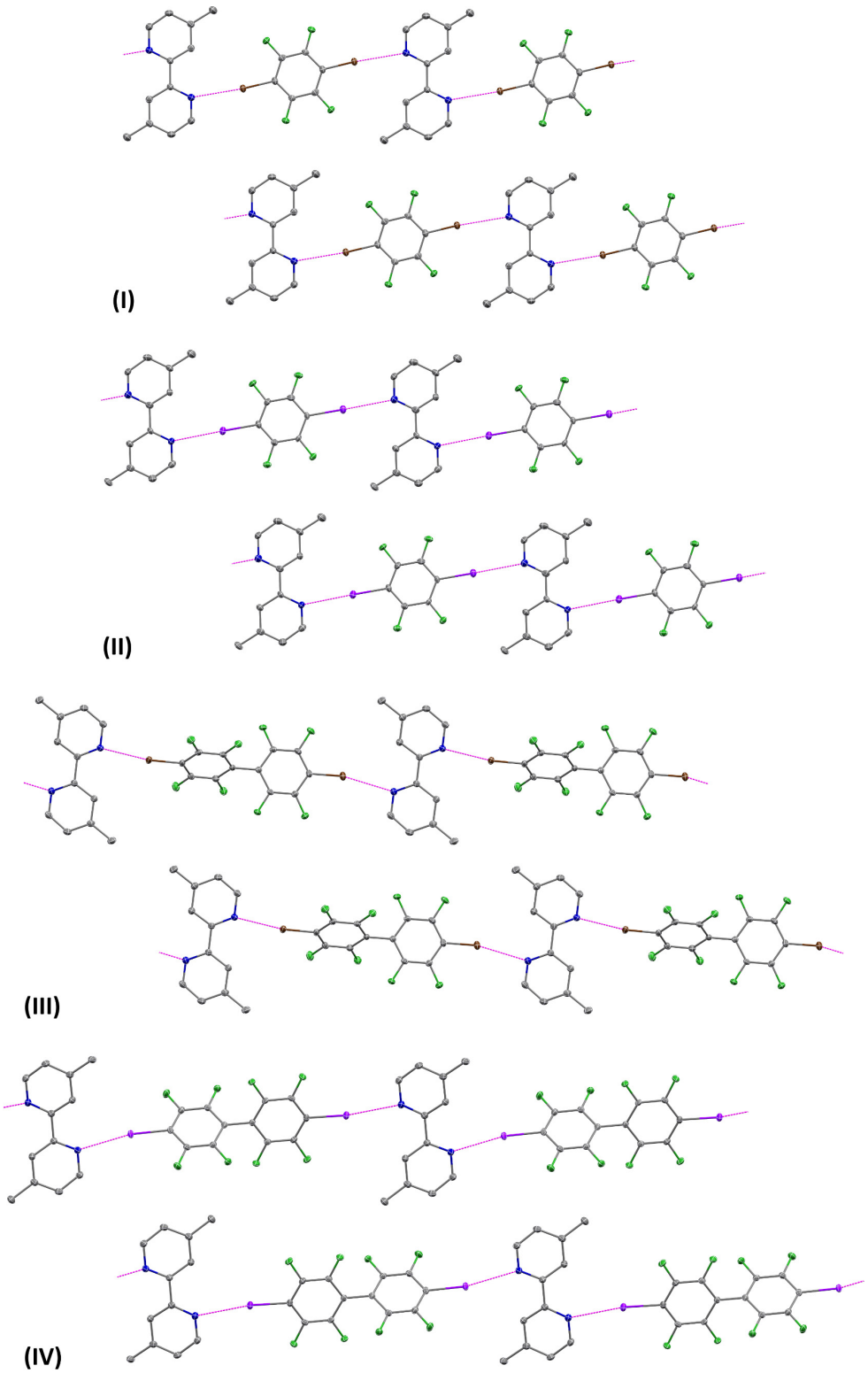

Figure SI33. Neighboring 1-d halogen bonding chains in (Br_2F_4bz)(4,4'-Me_2-2,2'-bipy) (I), (I_2F_4bz)(4,4'-Me_2-2,2'-bipy) (II), (Br_2F_8bph)(4,4'-Me_2-2,2'-bipy) (III), and (I_2F_8bph)(4,4'-Me_2-2,2'-bipy) (IV). Halogen bonds are shown as magenta dashed lines.

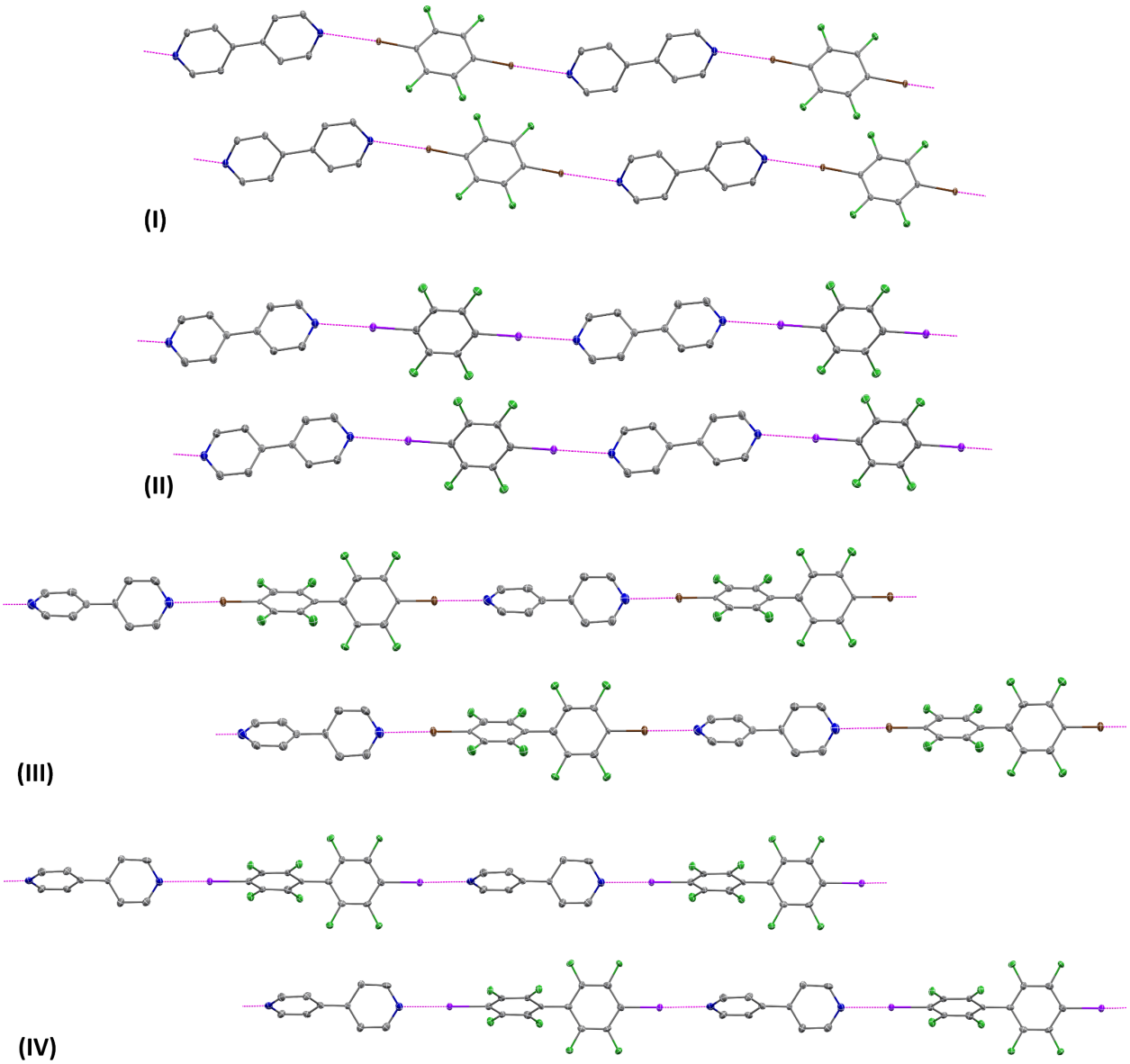

Figure SI34. Neighboring 1-d halogen bonding chains in (Br_2F_4bz)(4,4'-bipy) (I), (I_2F_4bz)(4,4'-bipy) (II), (Br_2F_8bph)(4,4'-bipy) (III), and (I_2F_8bph)(4,4'-bipy) (IV). Halogen bonds are shown as magenta dashed lines.

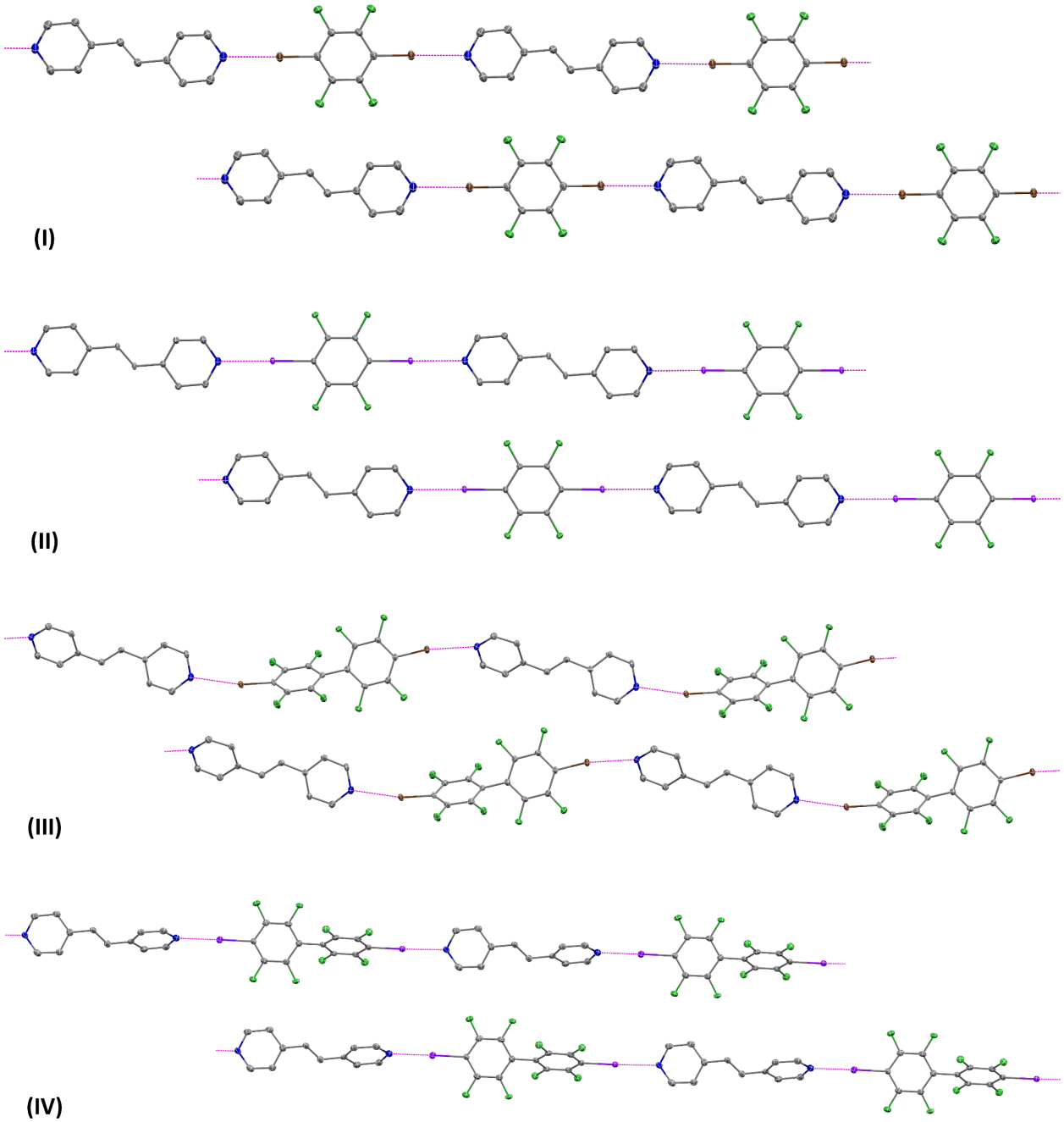

Figure SI35. Neighboring 1-d halogen bonding chains in (Br_2F_4bz)(dpe) (I), (I_2F_4bz)(dpe) (II), (Br_2F_8bph)(dpe) (III), and (I_2F_8bph)(dpe) (IV). Halogen bonds are shown as magenta dashed lines.

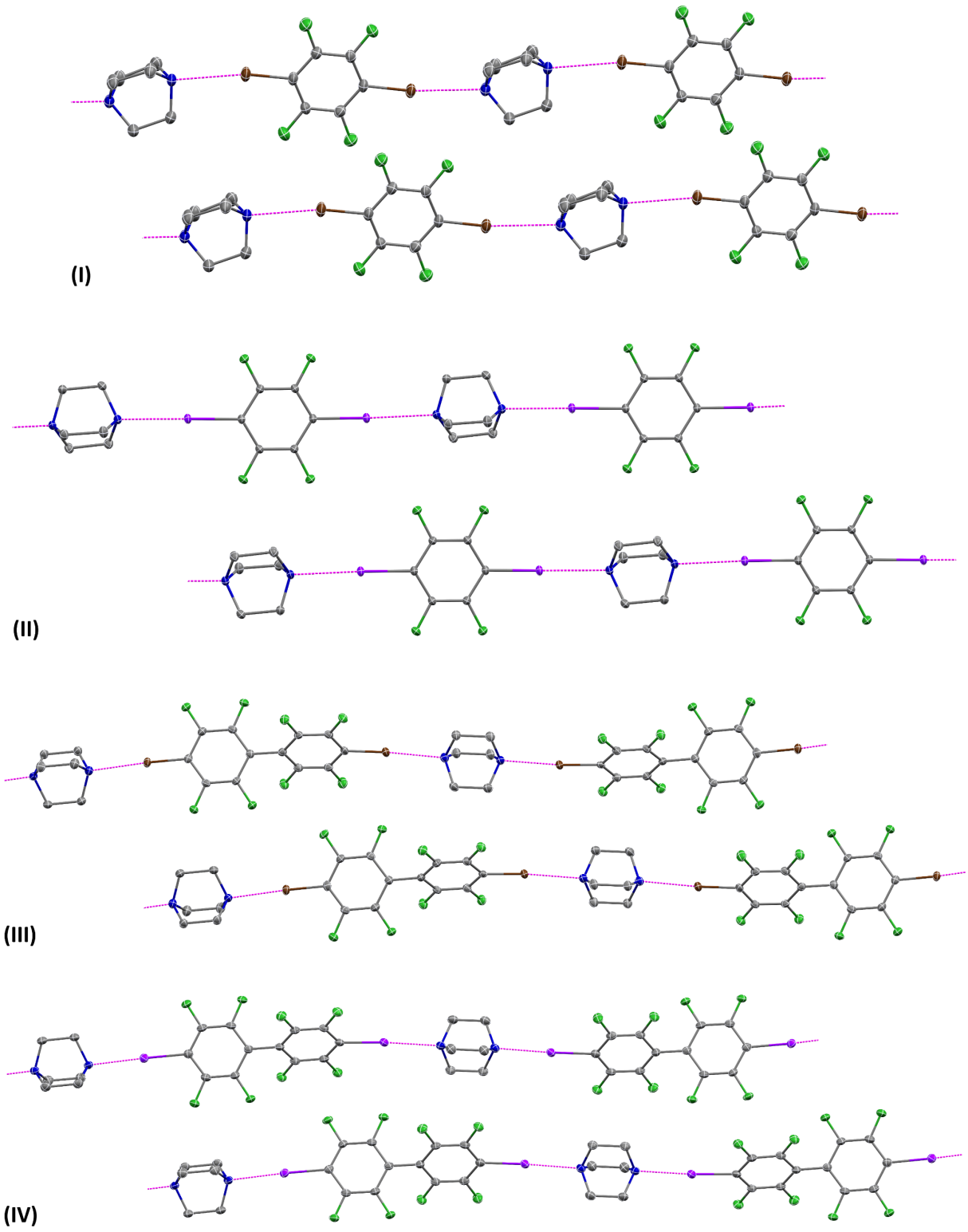

Figure SI36. Neighboring 1-d halogen bonding chains in (Br_2F_4bz)(DABCO) (I), (I_2F_4bz)(DABCO) (II), (Br_2F_8bph)(DABCO) (III), and (I_2F_8bph)(DABCO) (IV). Halogen bonds are shown as magenta dashed lines.

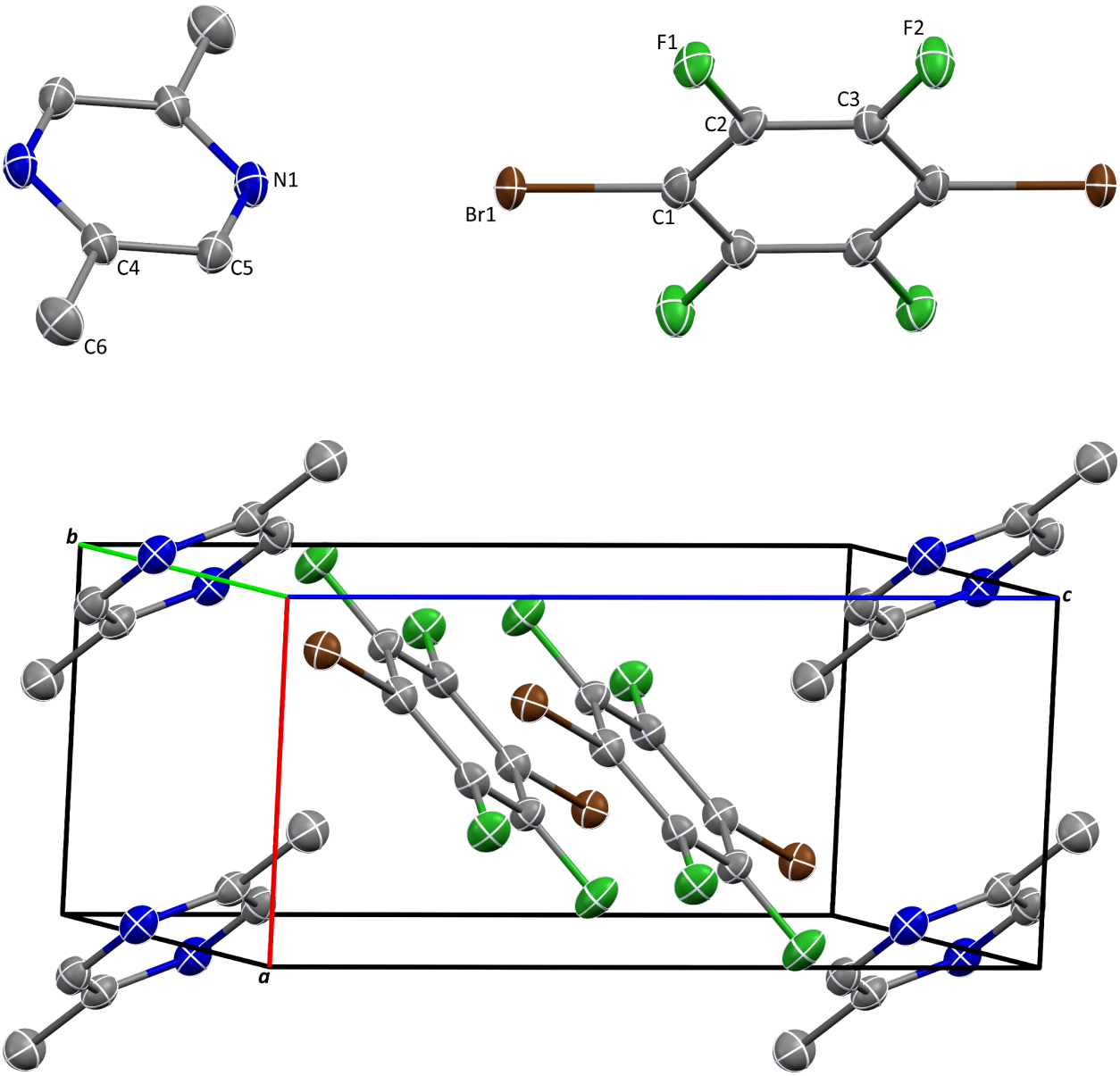

Figure SI37. Solid-state structure (top) and unit cell packing (bottom) of (Br_2F_4bz)(Me_2pyrz). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

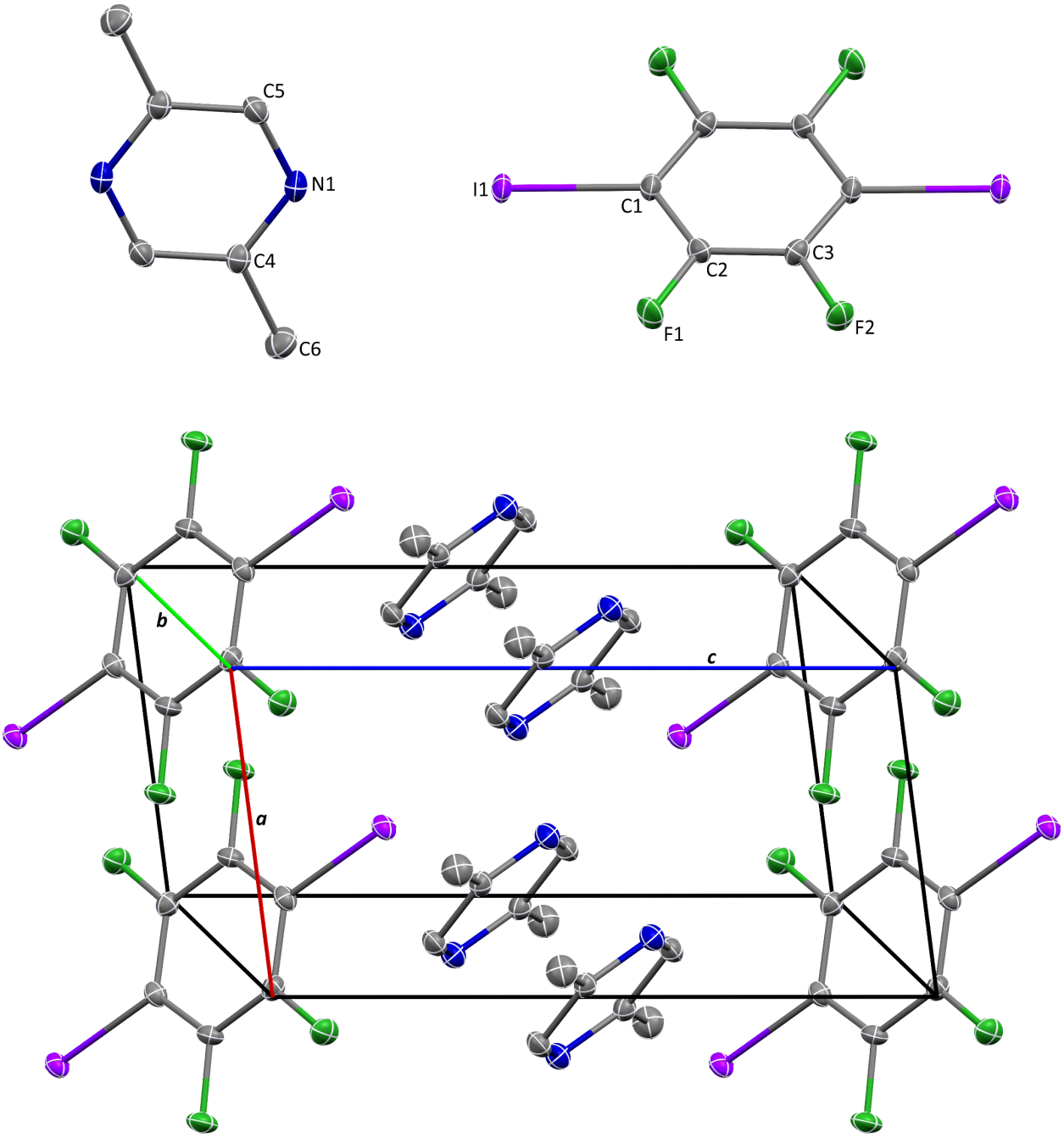

Figure SI38. Solid-state structure (top) and unit cell packing (bottom) of (I_2F_4bz)(Me_2pyrz). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

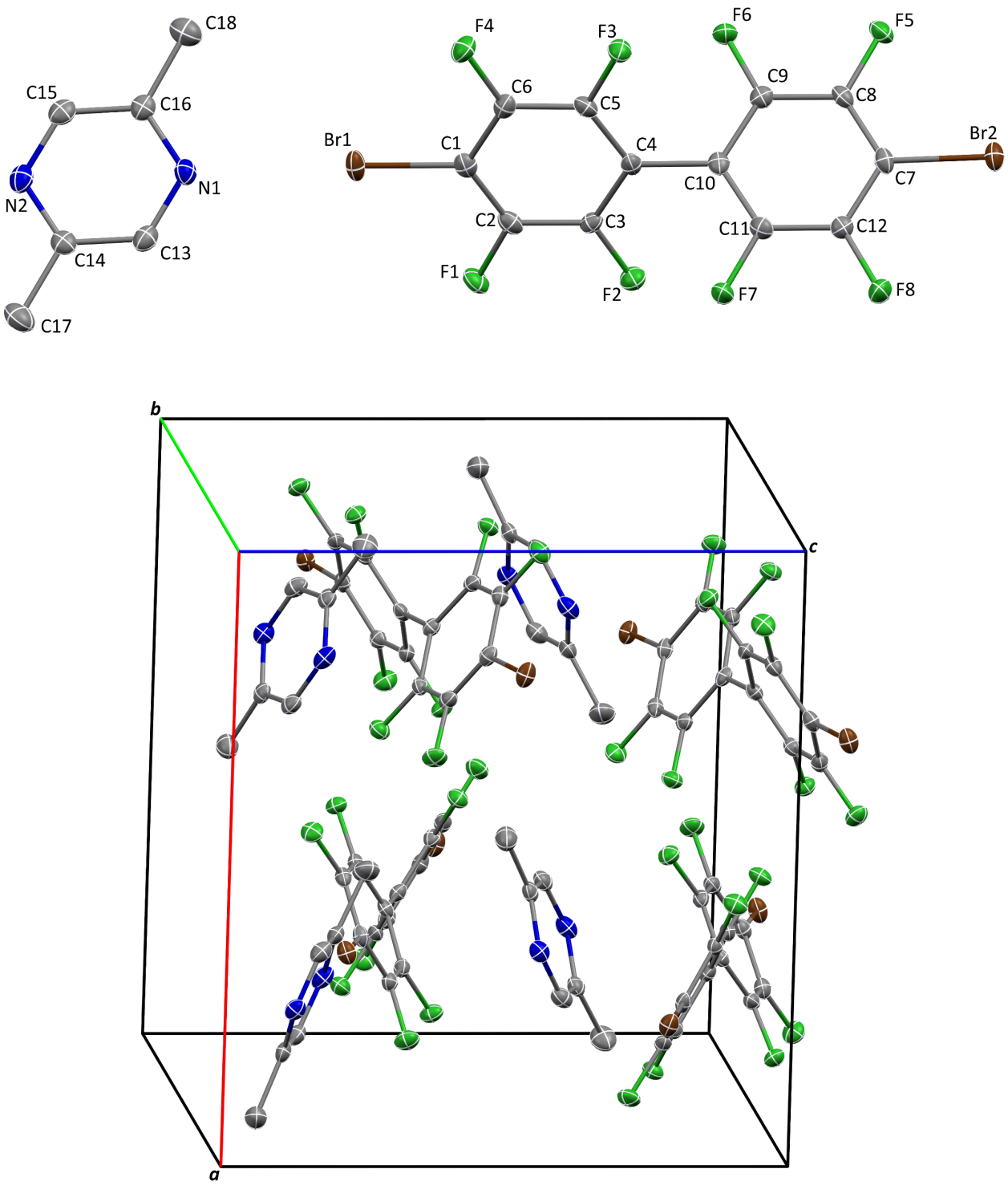

Figure SI39. Solid-state structure (top) and unit cell packing (bottom) of (Br_2F_8bph)(Me_2pyrz). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

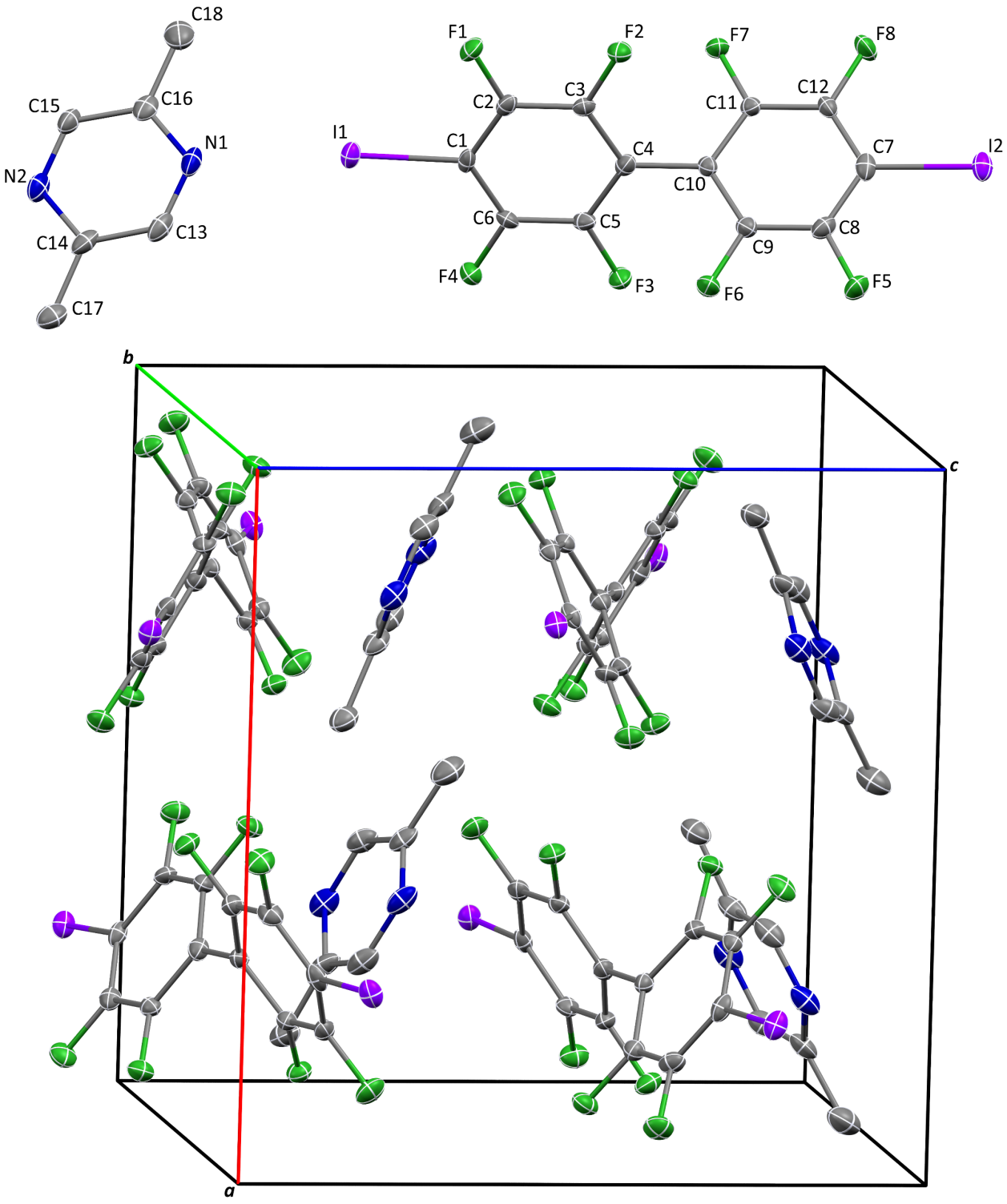

Figure SI40. Solid-state structure (top) and unit cell packing (bottom) of (I_2F_8bph)(Me_2pyrz). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

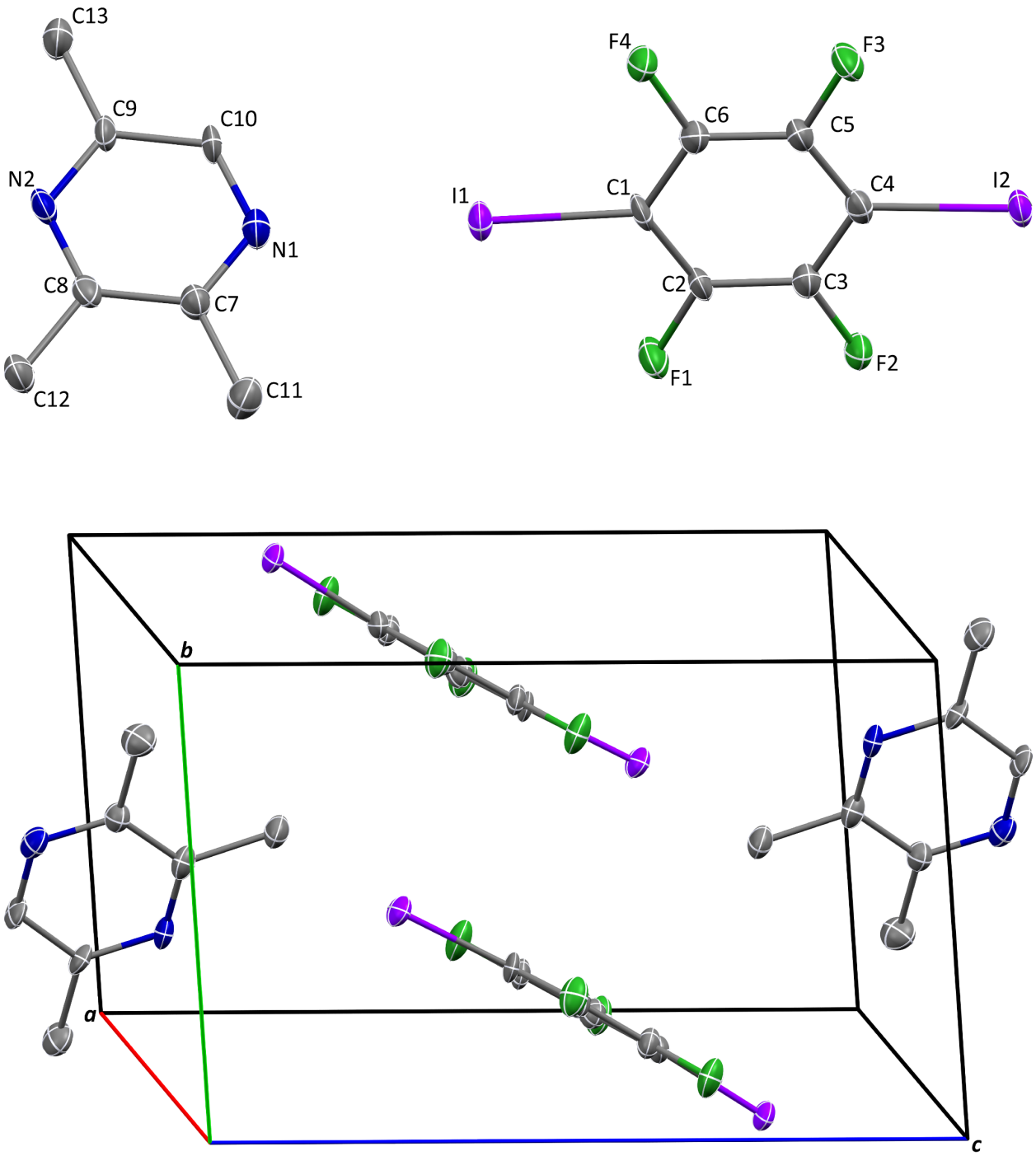

Figure SI41. Solid-state structure (top) and unit cell packing (bottom) of (I_2F_4bz)(Me_3pyrz). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

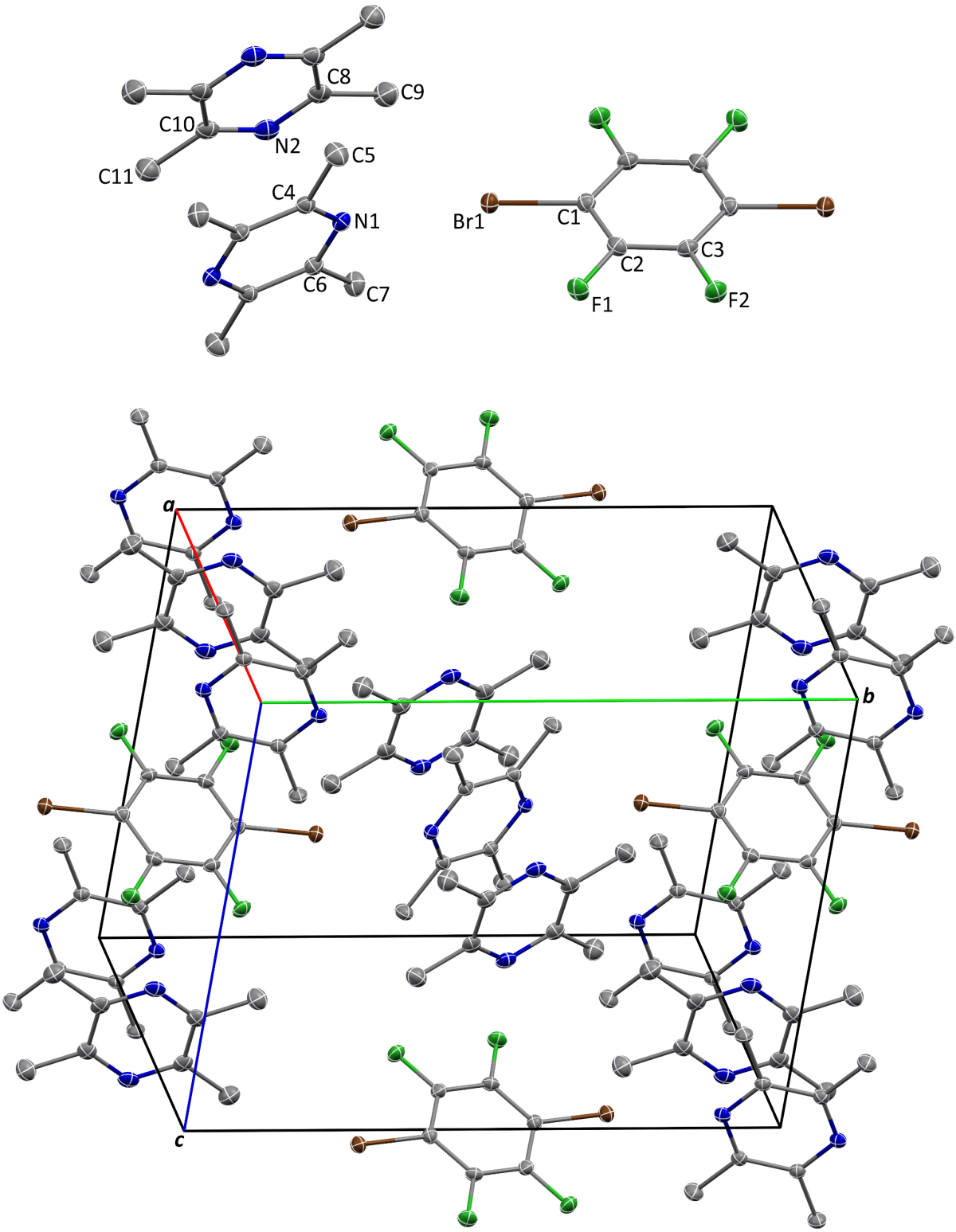

Figure SI42. Solid-state structure (top) and unit cell packing (bottom) of $(Br_2F_4bz)2(Me_4pyrz)$. Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

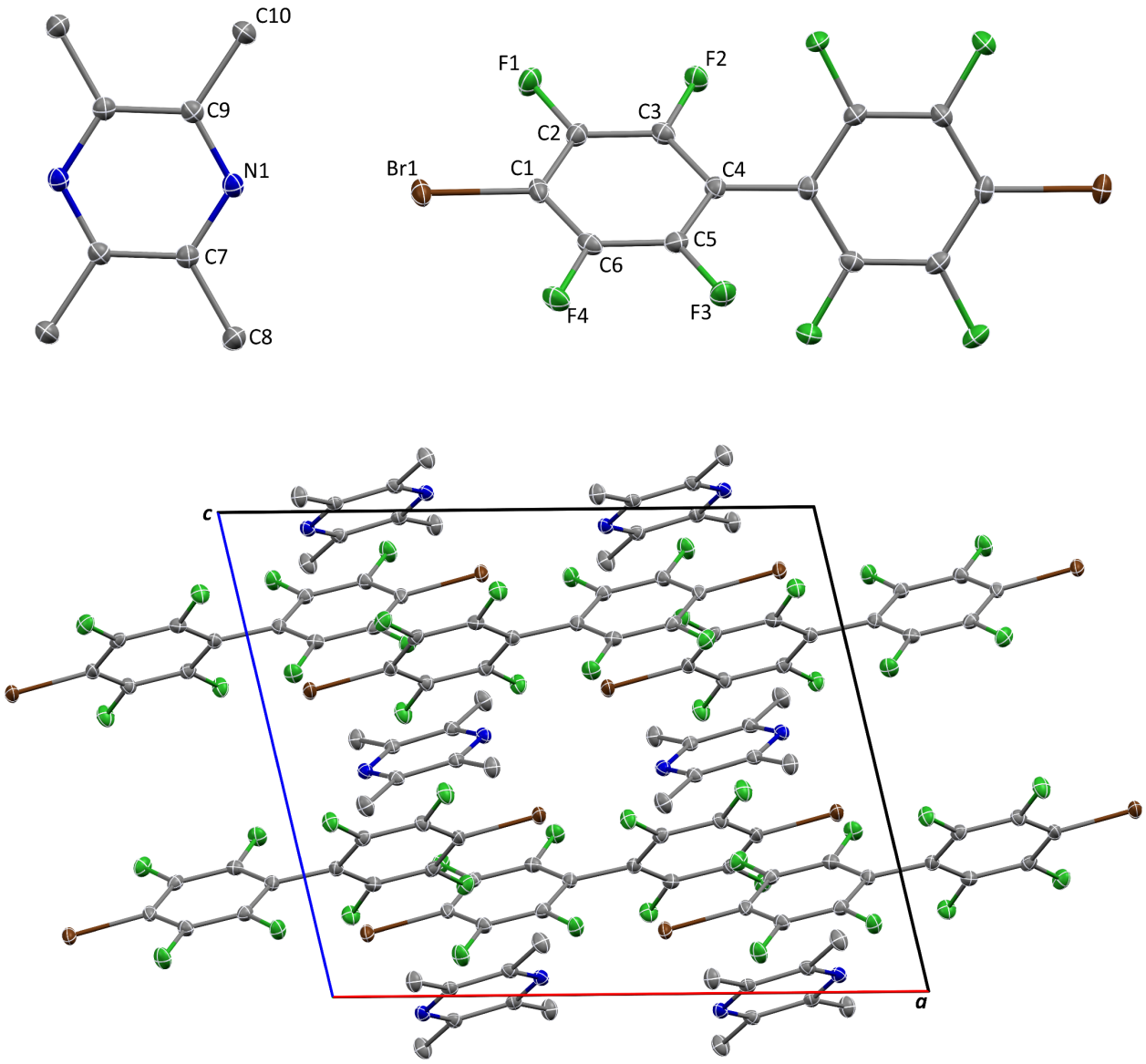

Figure SI43. Solid-state structure (top) and unit cell packing (bottom, viewed down the *b* axis) of (Br_2F_8bph)(Me_4pyrz). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

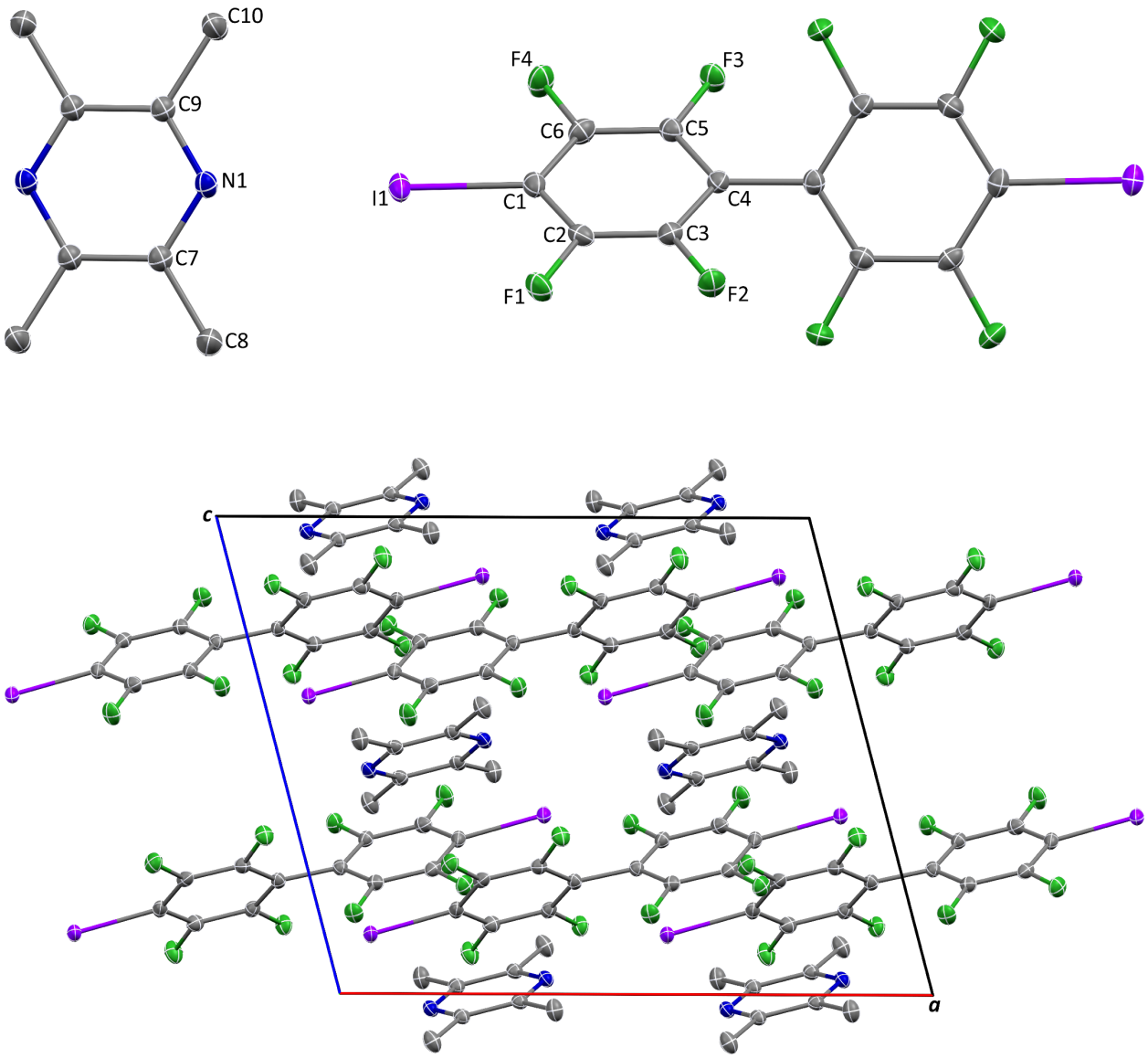

Figure SI44. Solid-state structure (top) and unit cell packing (bottom, viewed down the *b* axis) of (I_2F_8bph)(Me_4pyrz). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

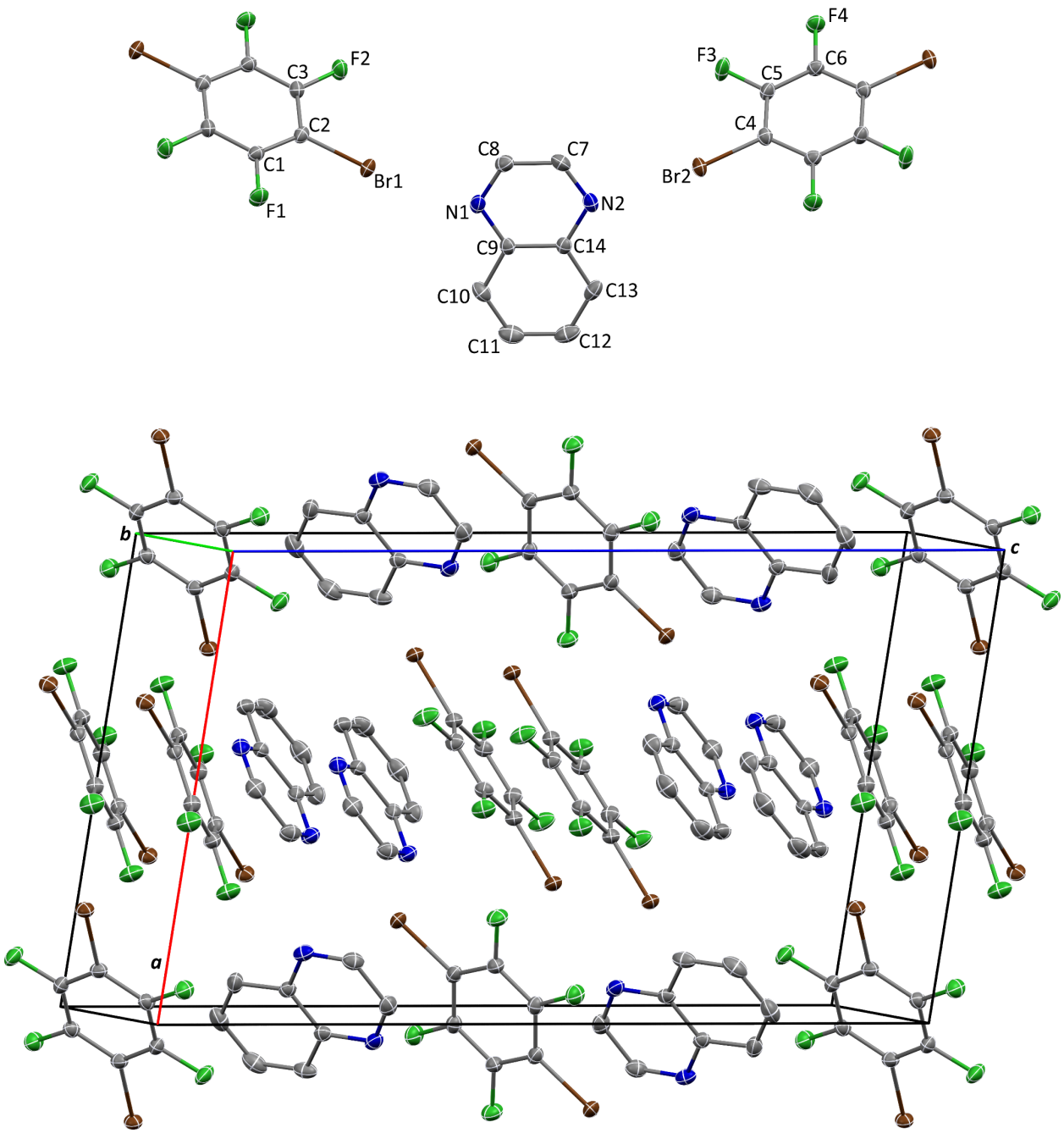

Figure SI45. Solid-state structure (top) and unit cell packing (bottom) of (Br_2F_4bz)(quinox). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

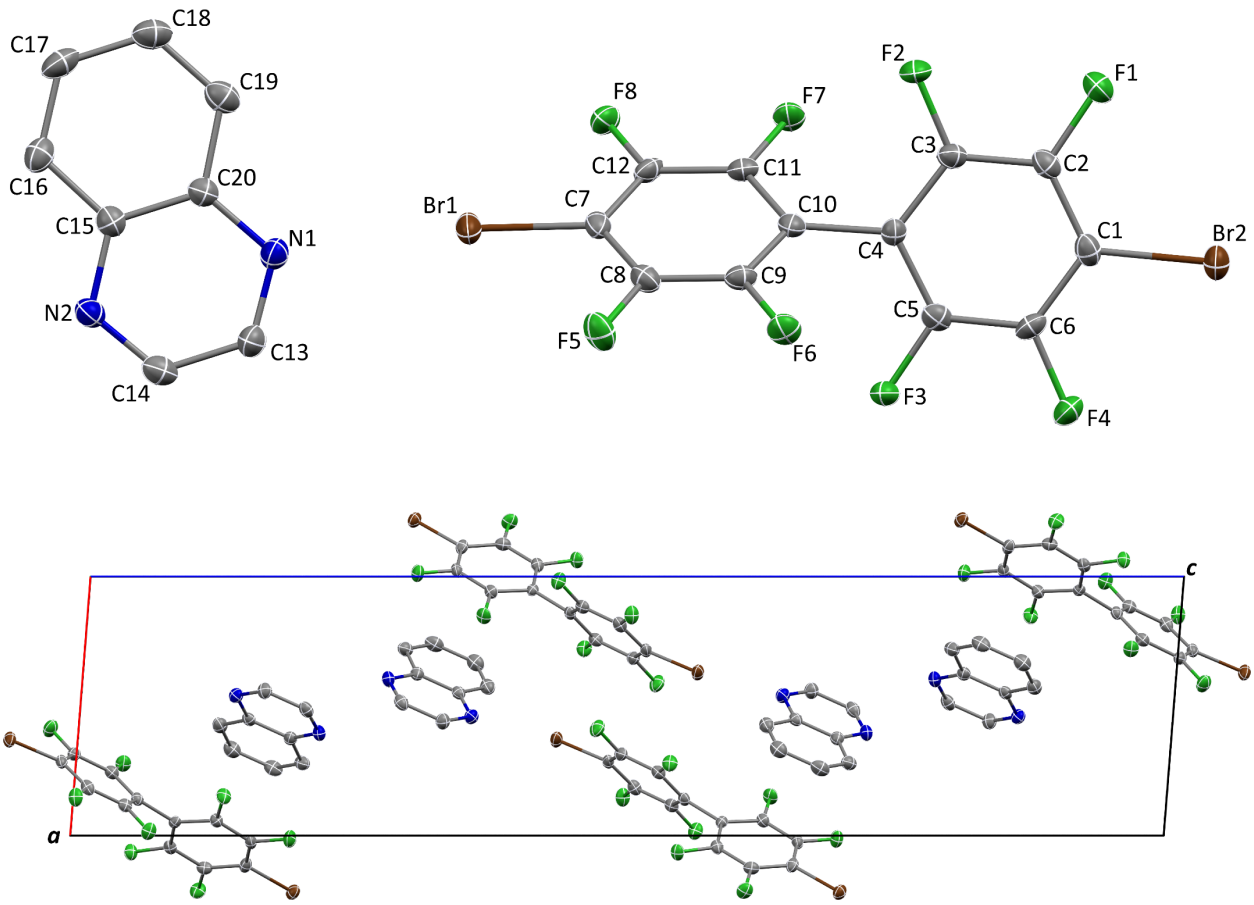

Figure SI46. Solid-state structure (top) and unit cell packing (bottom, viewed down the *b* axis) of (Br_2F_8bph)(quinox). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

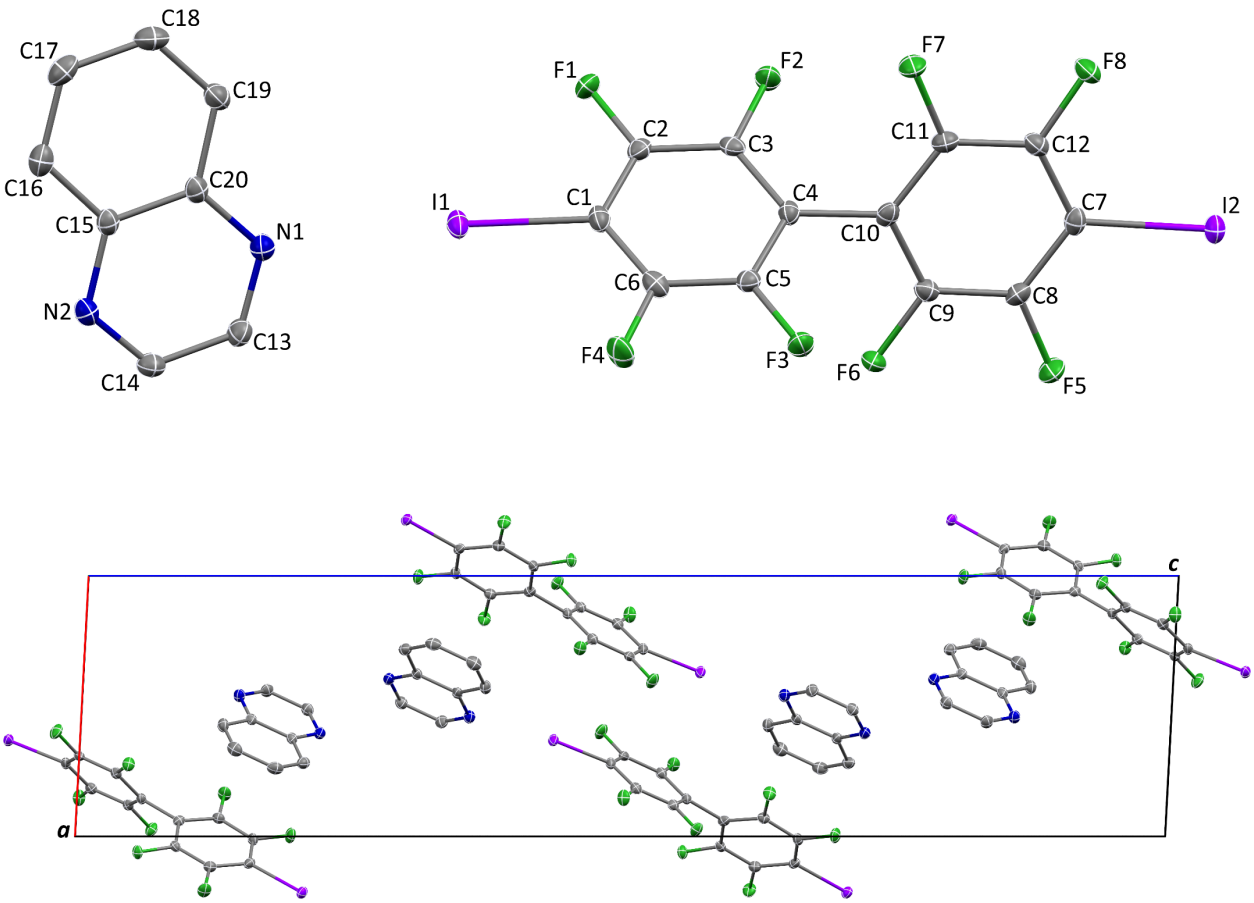

Figure SI47. Solid-state structure (top) and unit cell packing (bottom, viewed down the *b* axis) of (I_2F_8bph)(quinox). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

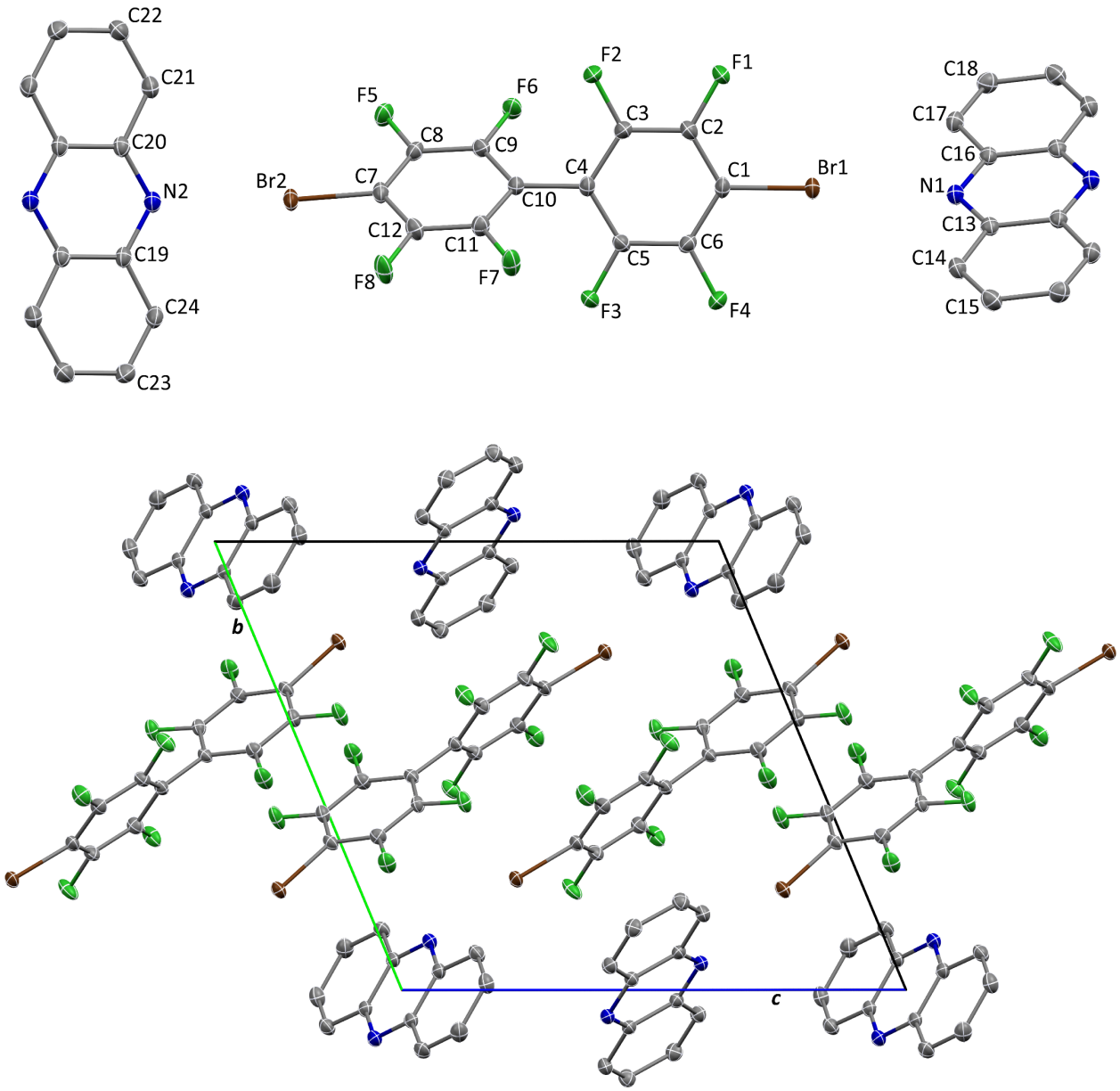

Figure SI48. Solid-state structure (top) and unit cell packing (bottom, viewed down the *a* axis) of (Br_2F_8bph)(phenaz). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

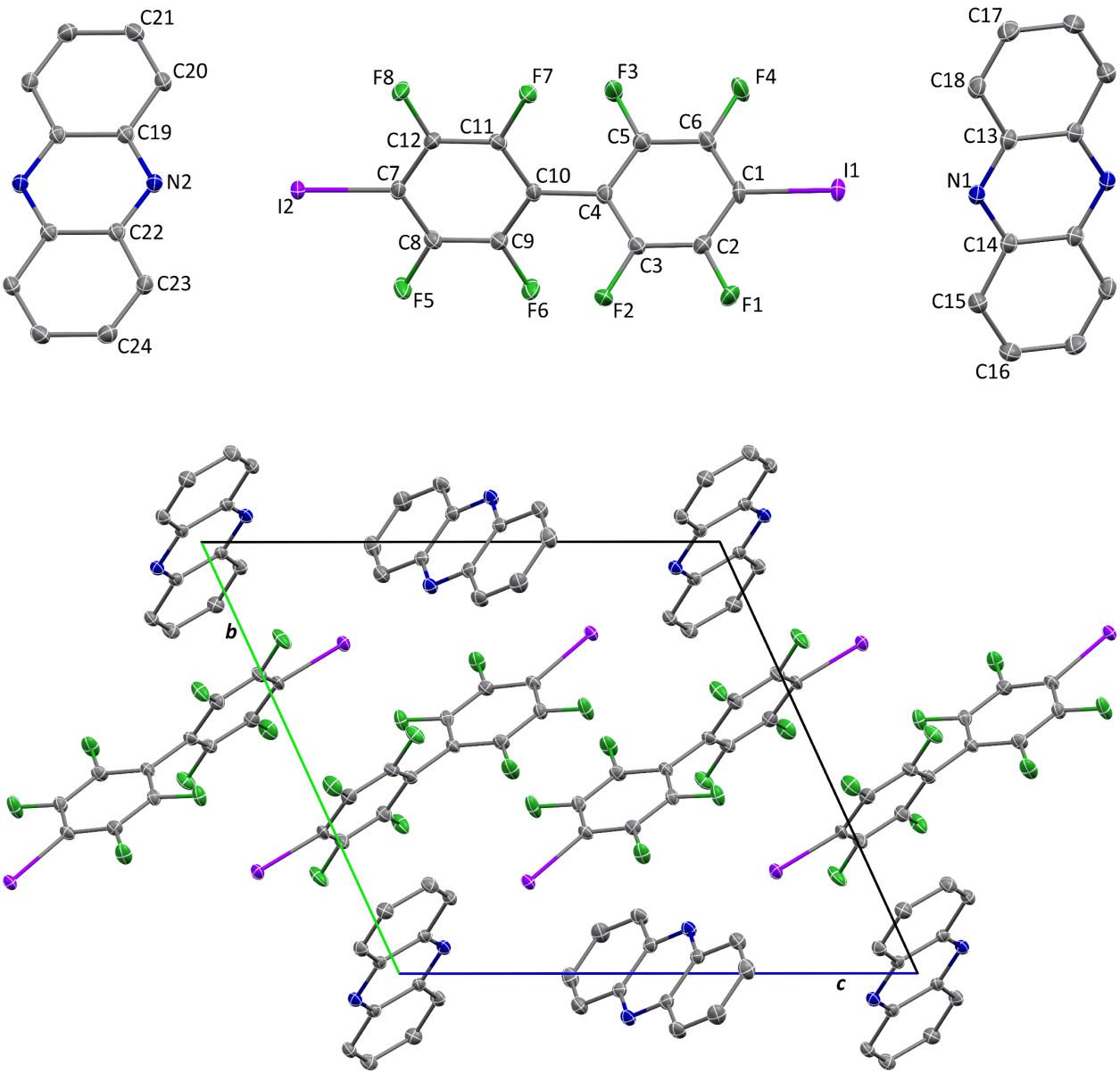

Figure SI49. Solid-state structure (top) and unit cell packing (bottom, viewed down the *a* axis) of (I_2F_8bph)(phenaz). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

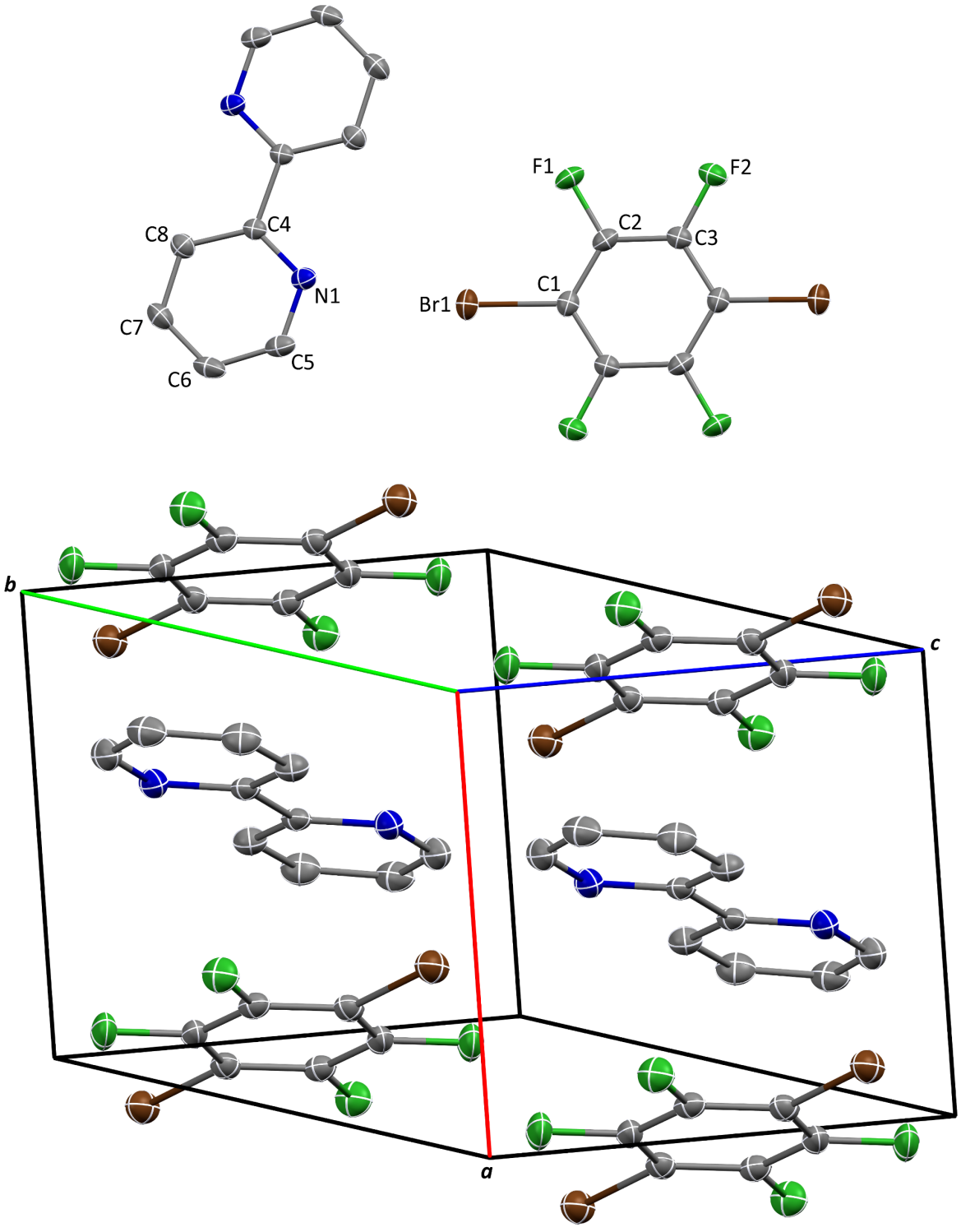

Figure SI50. Solid-state structure (top) and unit cell packing (bottom) of (Br_2F_4bz)(2,2'-bipy). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

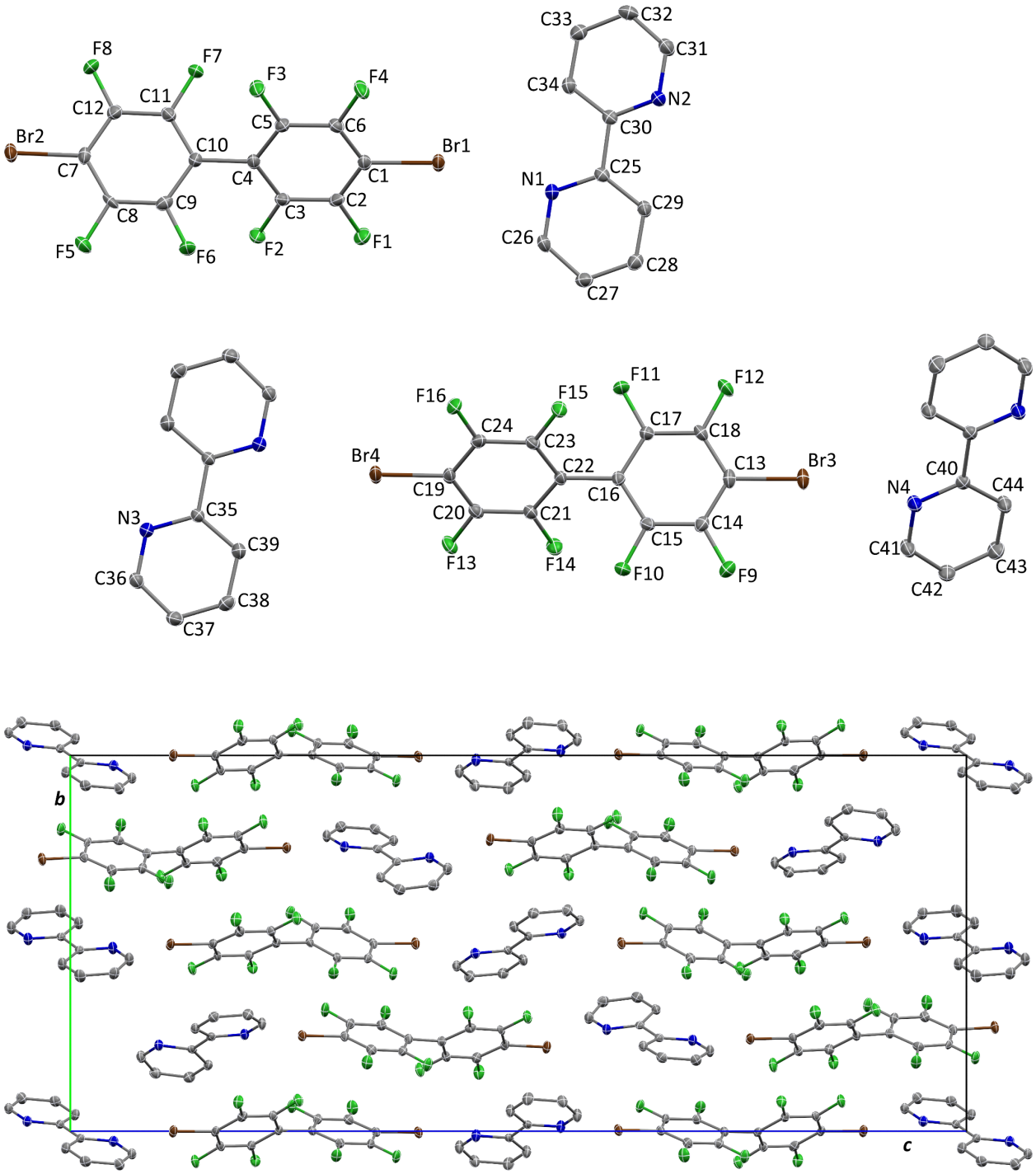

Figure SI51. Solid-state structure (top) and unit cell packing (bottom, viewed down the *a* axis) of (Br_2F_8bph)(2,2'-bipy). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

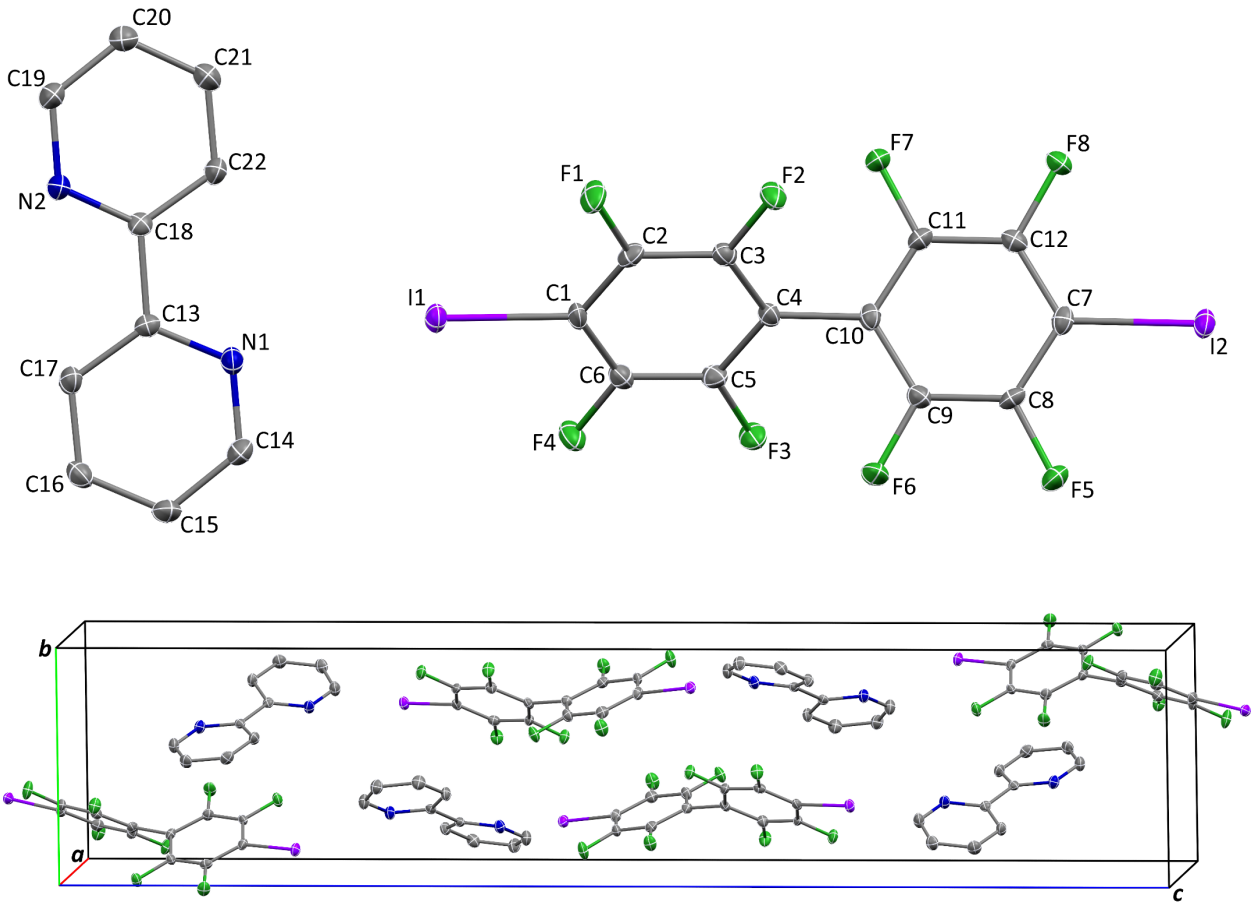

Figure SI52. Solid-state structure (top) and unit cell packing (bottom) of (I_2F_8bph)(2,2'-bipy). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

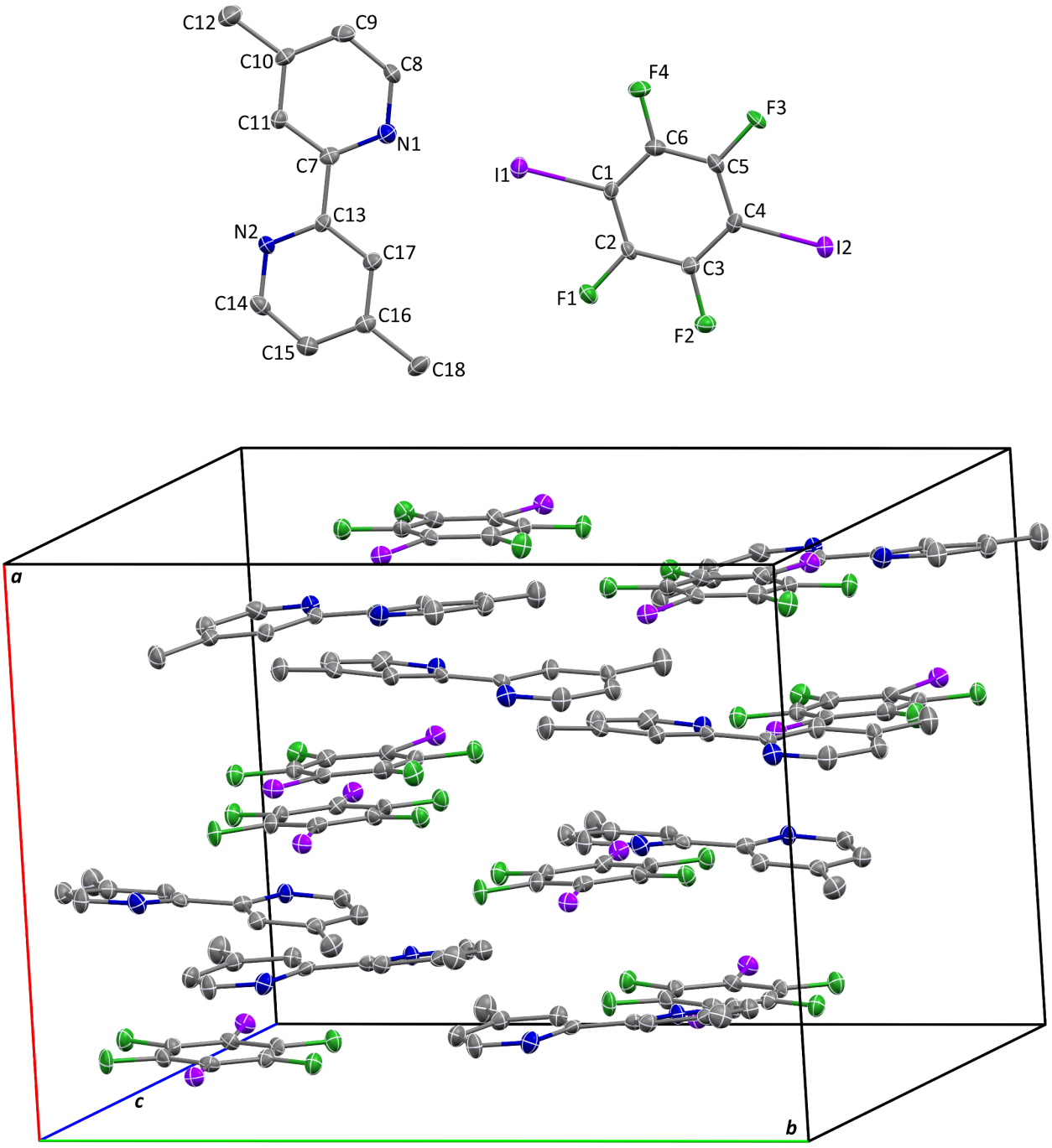

Figure SI53. Solid-state structure (top) and unit cell packing (bottom) of (I_2F_4bz)(4,4'-Me2-2,2'-bipy). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

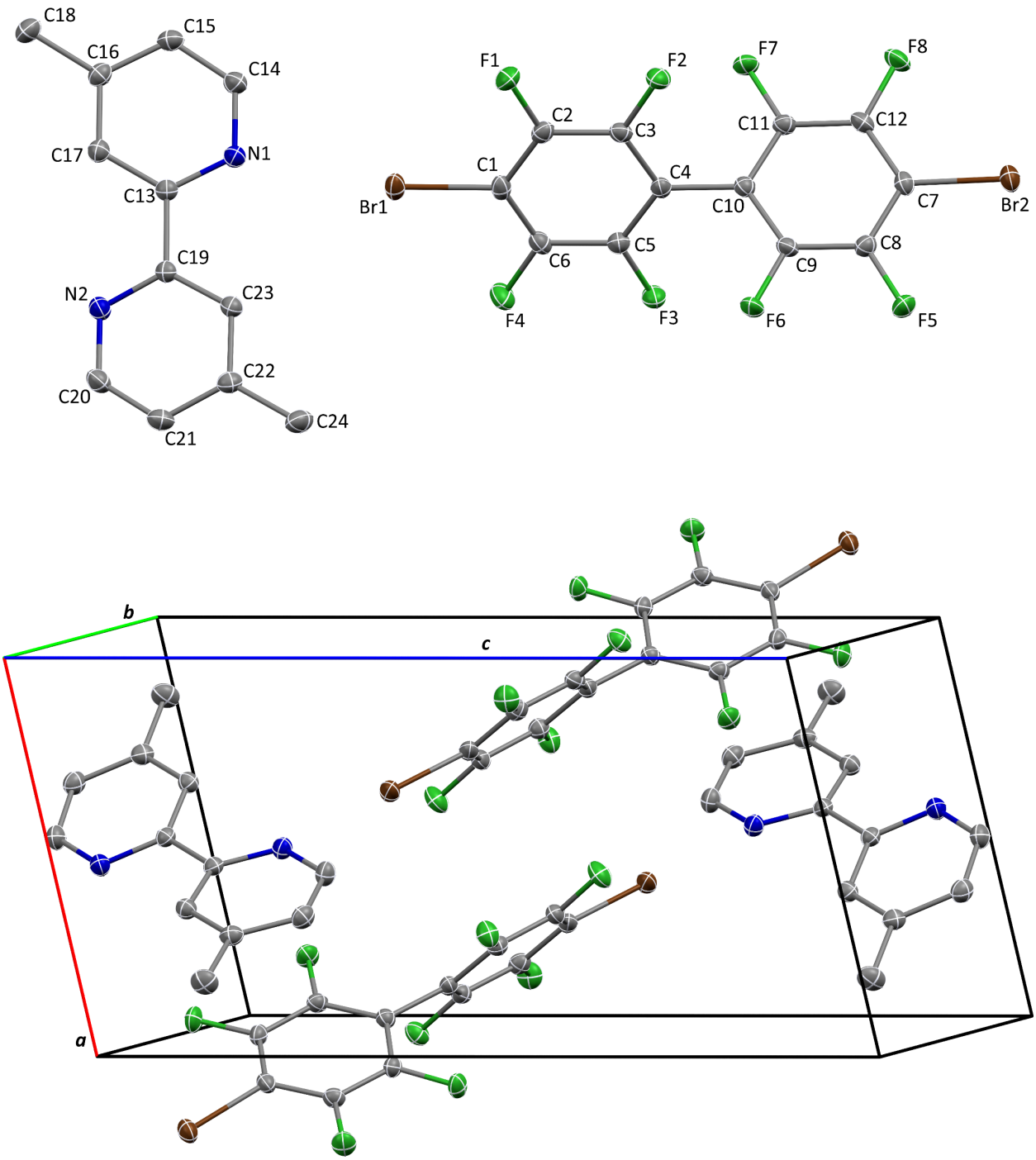

Figure SI54. Solid-state structure (top) and unit cell packing (bottom) of (Br_2F_8bph)(4,4'-Me2-2,2'-bipy). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

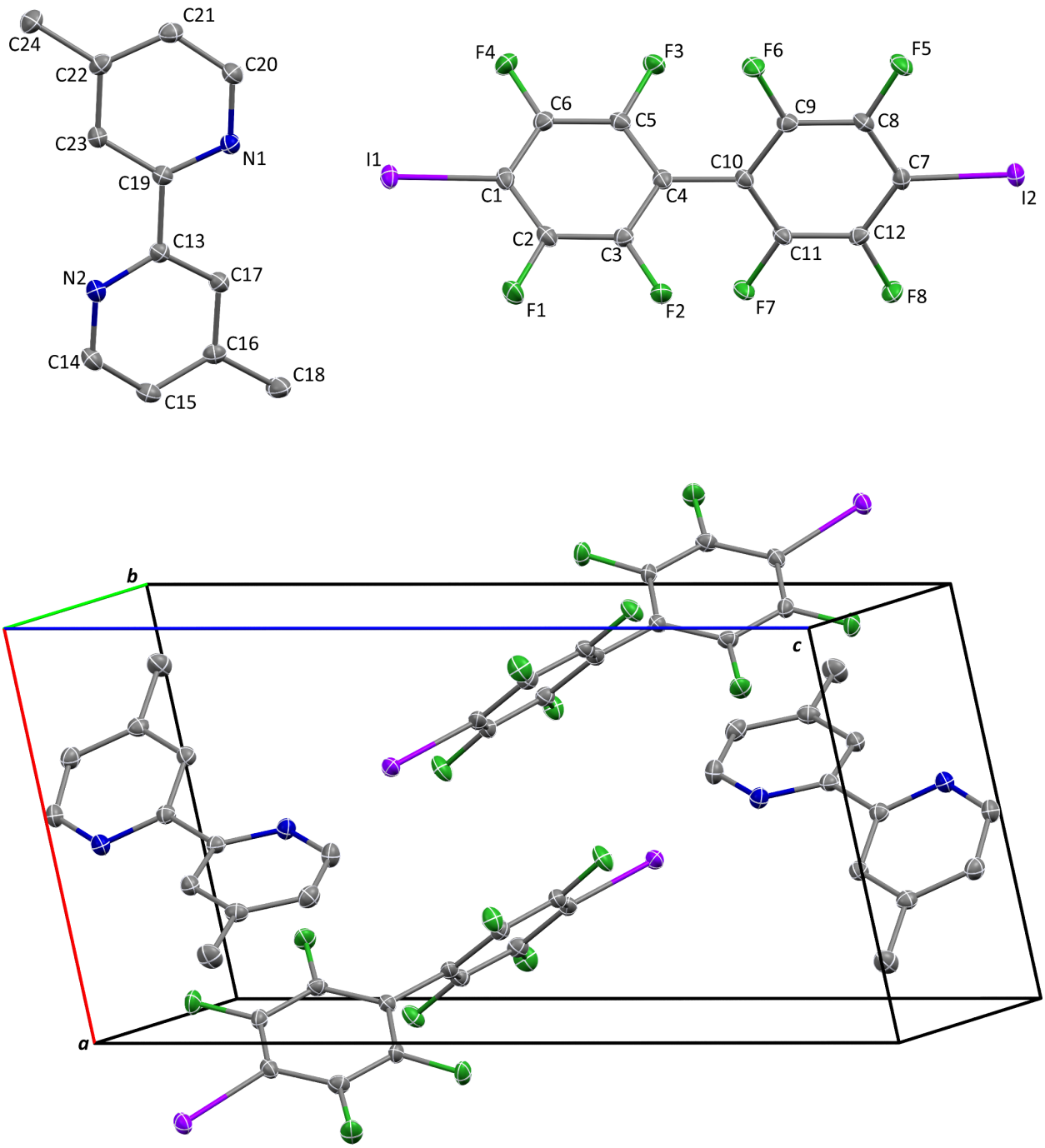

Figure SI55. Solid-state structure (top) and unit cell packing (bottom) of (I_2F_8bph)(4,4'-Me2-2,2'-bipy). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

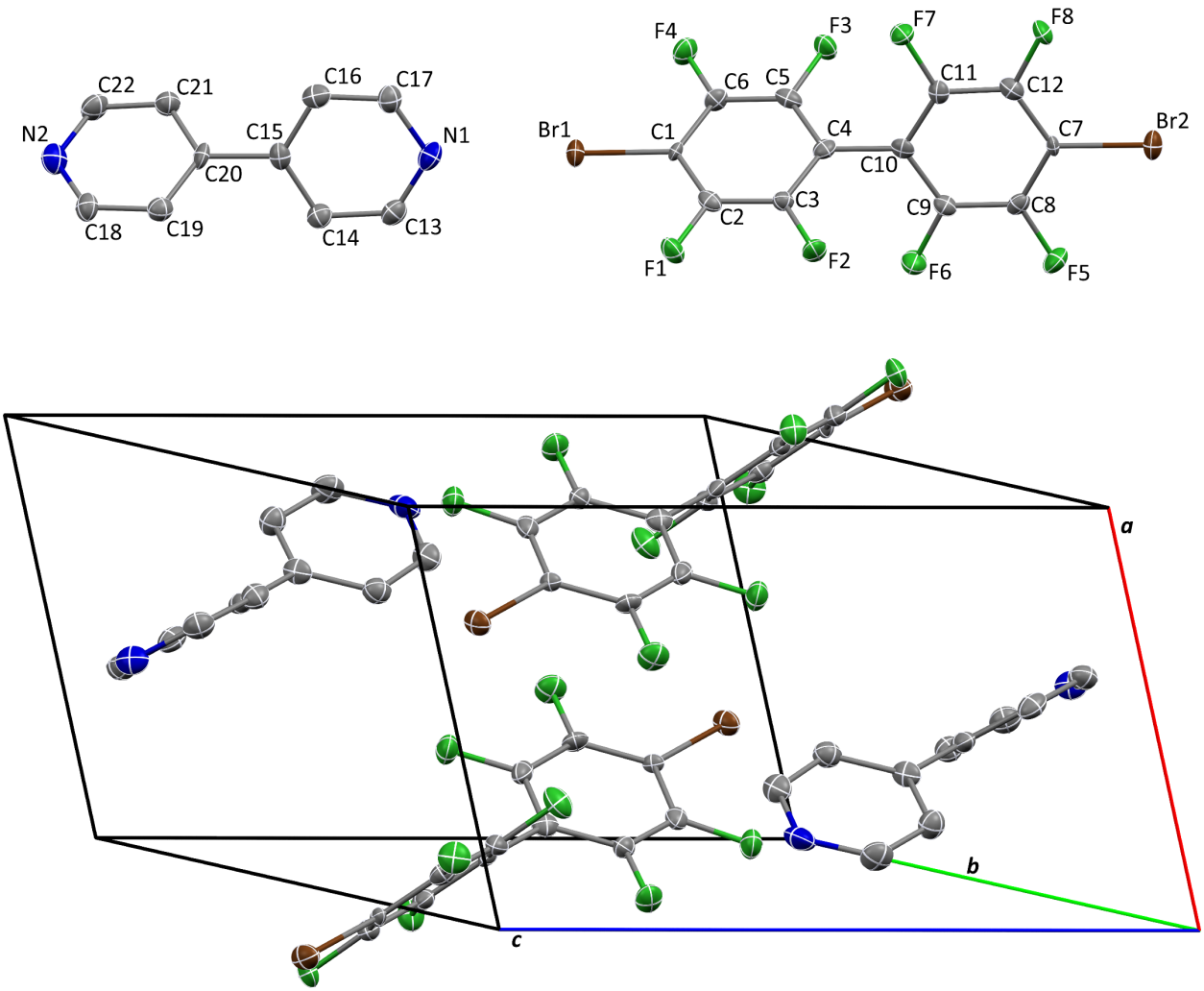

Figure SI56. Solid-state structure (top) and unit cell packing (bottom) of (Br_2F_8bph)(4,4'-bipy). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

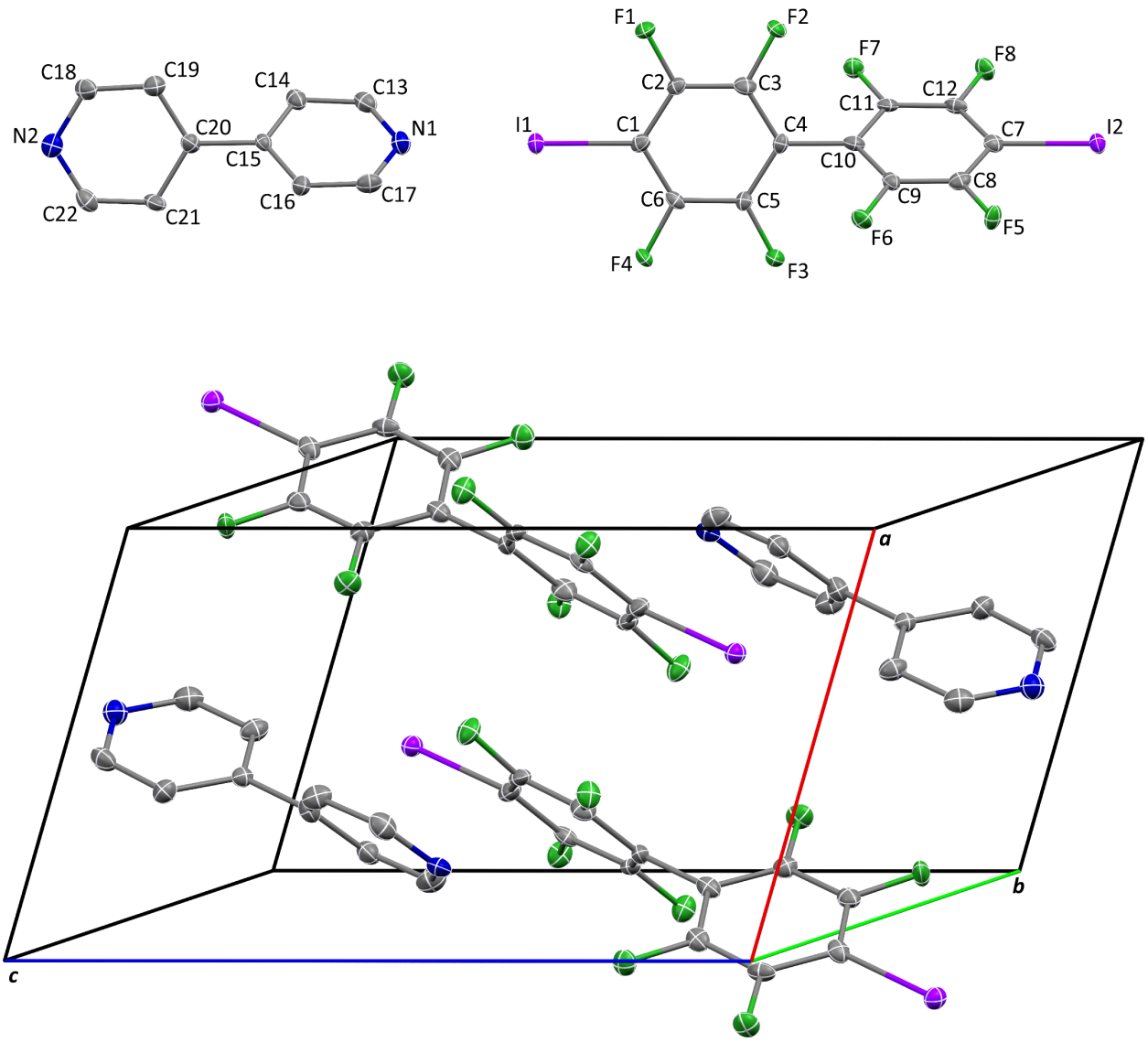

Figure SI57. Solid-state structure (top) and unit cell packing (bottom) of (I_2F_8bph)(4,4'-bipy). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

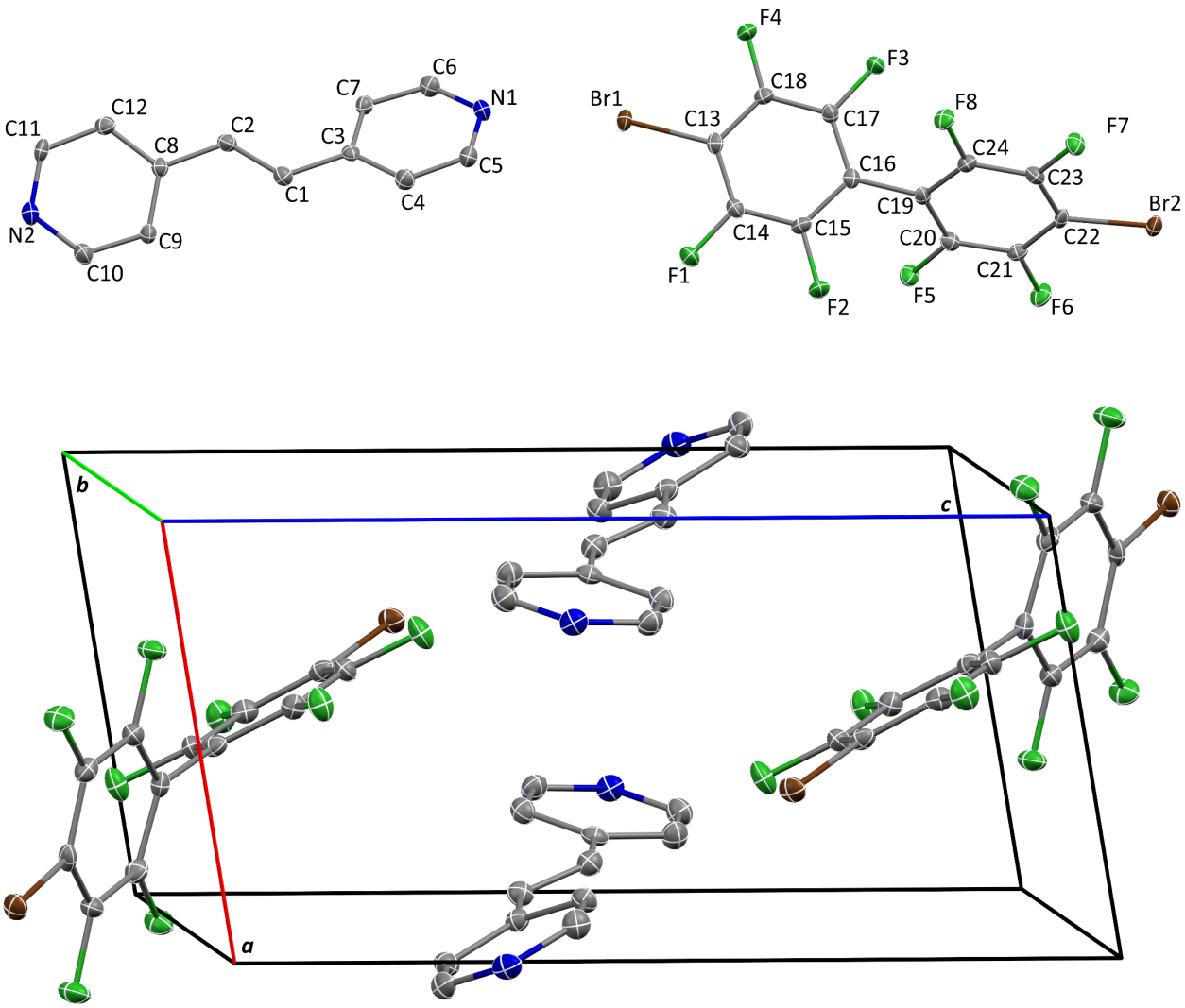

Figure SI58. Solid-state structure (top) and unit cell packing (bottom) of (Br_2F_8bph)(dpe). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

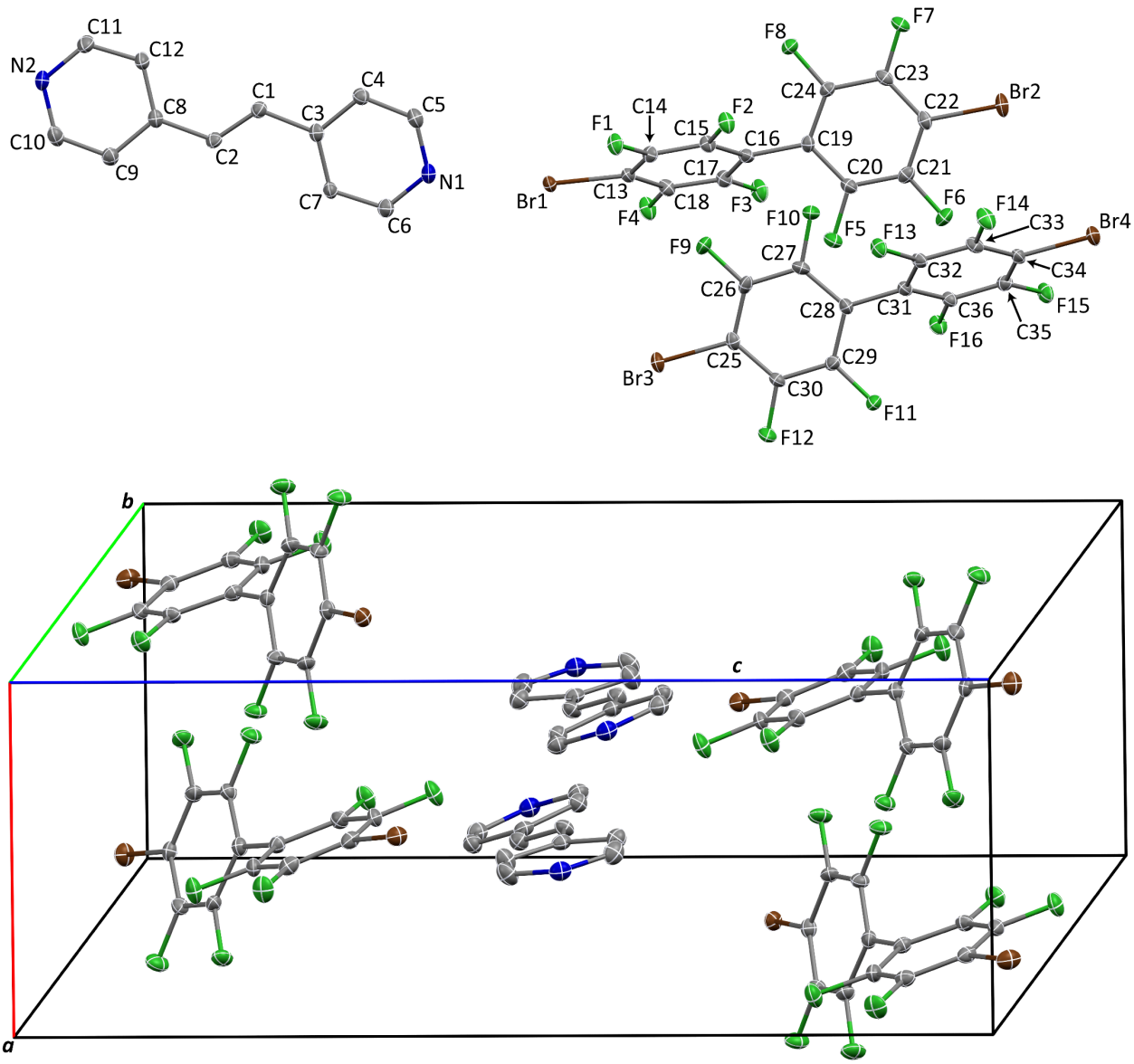

Figure SI59. Solid-state structure (top) and unit cell packing (bottom) of 2(Br_2F_8bph)(dpe). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

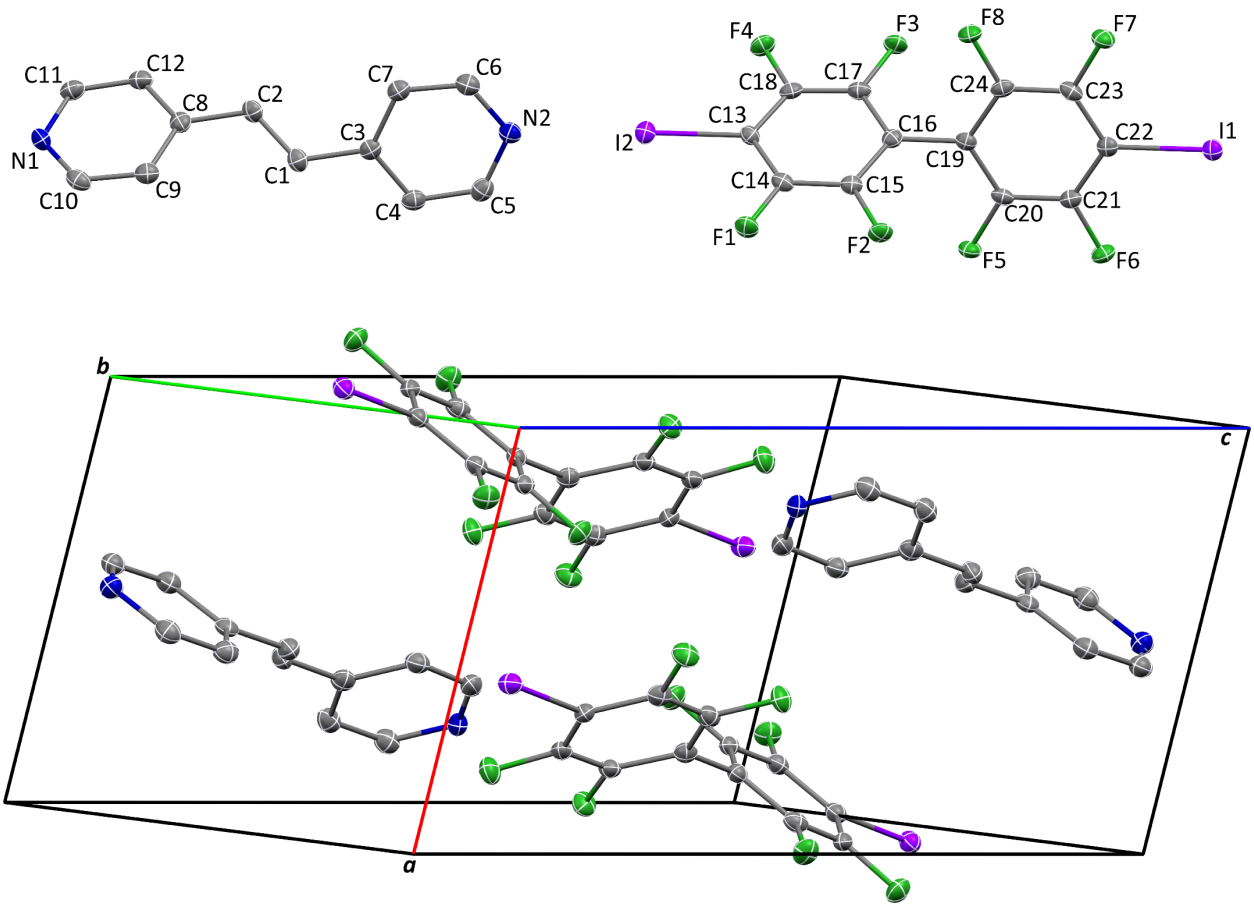

Figure SI60. Solid-state structure (top) and unit cell packing (bottom) of (I_2F_8bph)(dpe). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

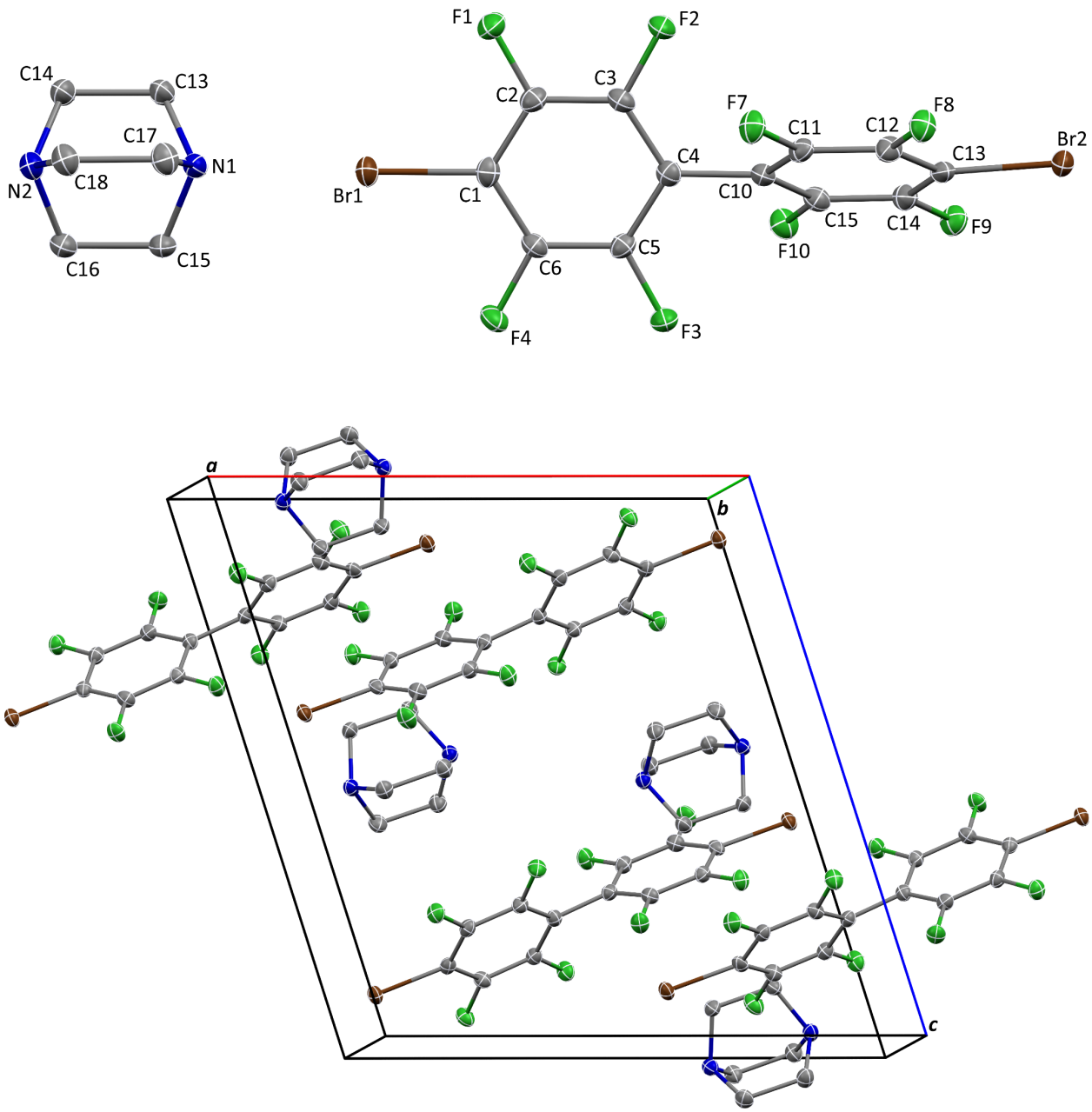

Figure SI61. Solid-state structure (top) and unit cell packing (bottom) of (Br_2F_8bph)(DABCO). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

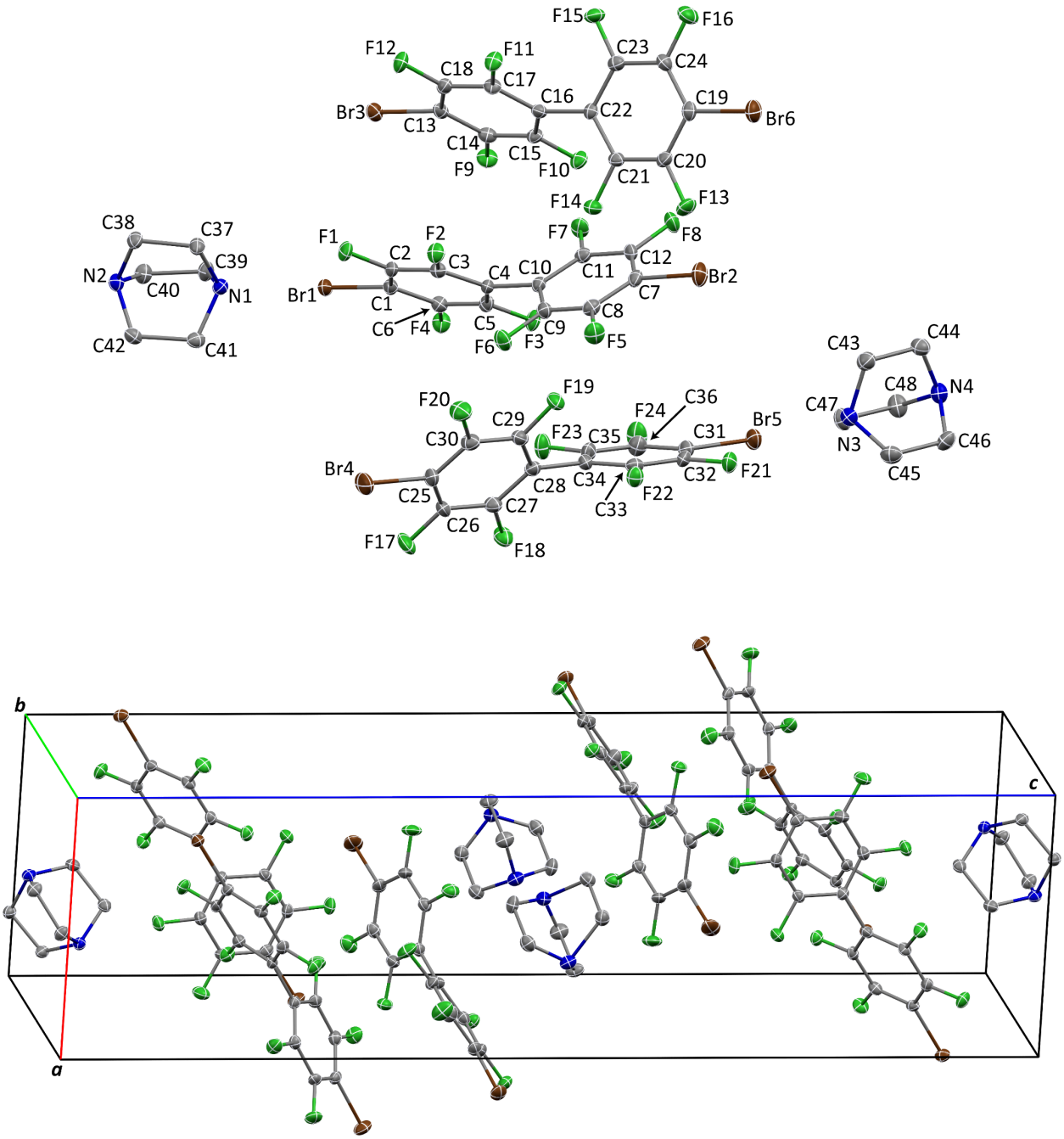

Figure SI62. Solid-state structure (top) and unit cell packing (bottom) of $(Br_2F_8bph)_2$(DABCO). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

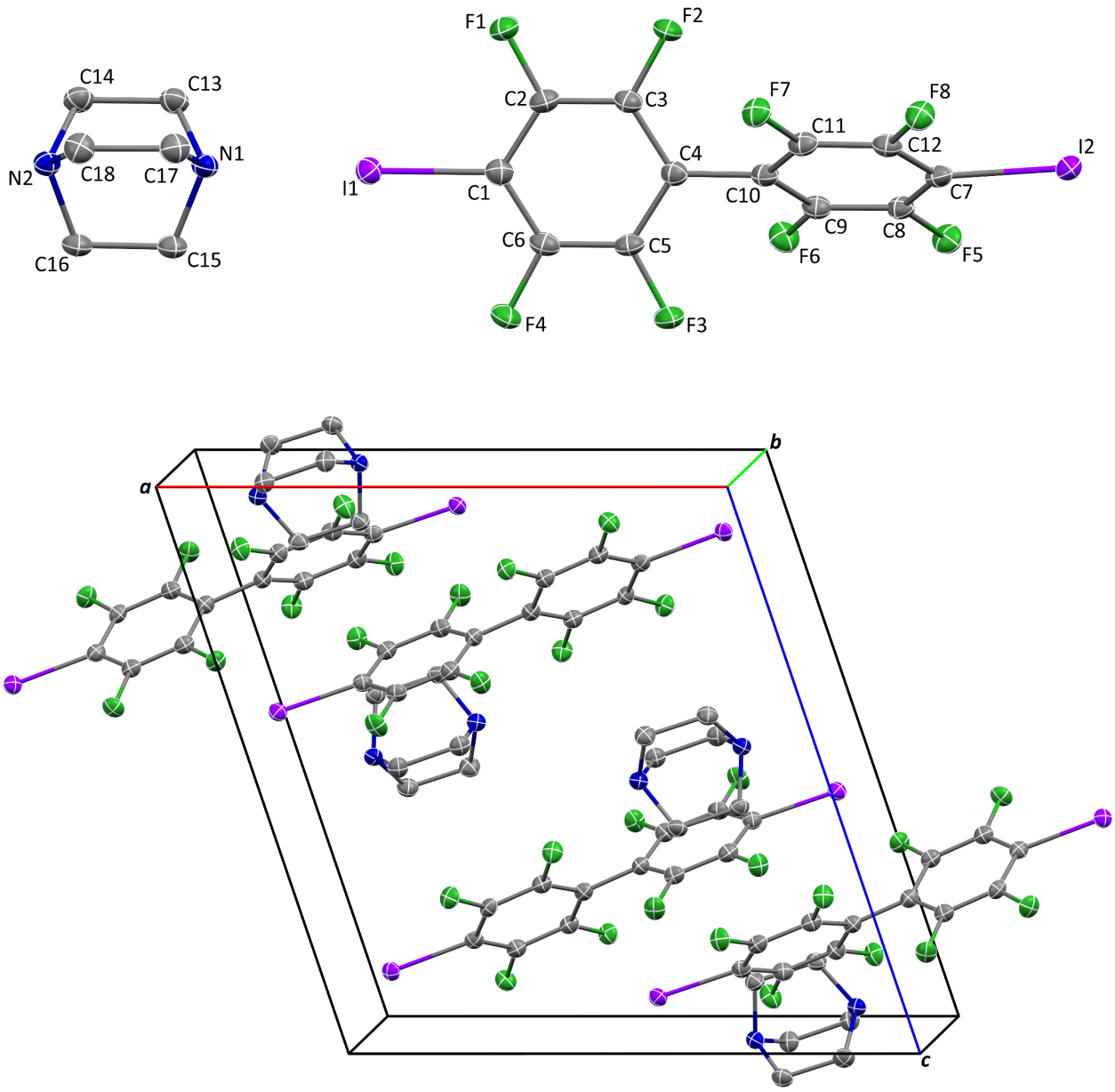

Figure SI63. Solid-state structure (top) and unit cell packing (bottom) of (I_2F_8bph)(DABCO). Atomic displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms have been omitted for clarity.

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