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Supporting information for article:

^{13}C and ^{19}F solid-state NMR and X-ray crystallographic study of halogen-bonded frameworks featuring nitrogen-containing heterocycles

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Supporting Information

^{13}C and ^{19}F Solid-State NMR and X-Ray Crystallographic Study of Halogen-Bonded Frameworks Featuring Nitrogen-Containing Heterocycles

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Contents

List of Figures

List of Tables

Powder X-ray Diffraction

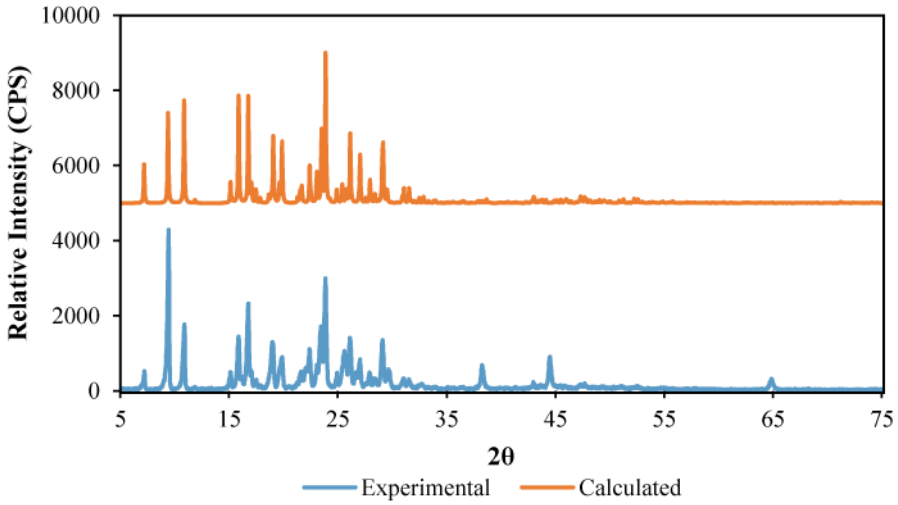

Figure S1. Powder X-ray diffraction pattern of **A** (acridine, ACD), with the calculated diffraction pattern overlaid.

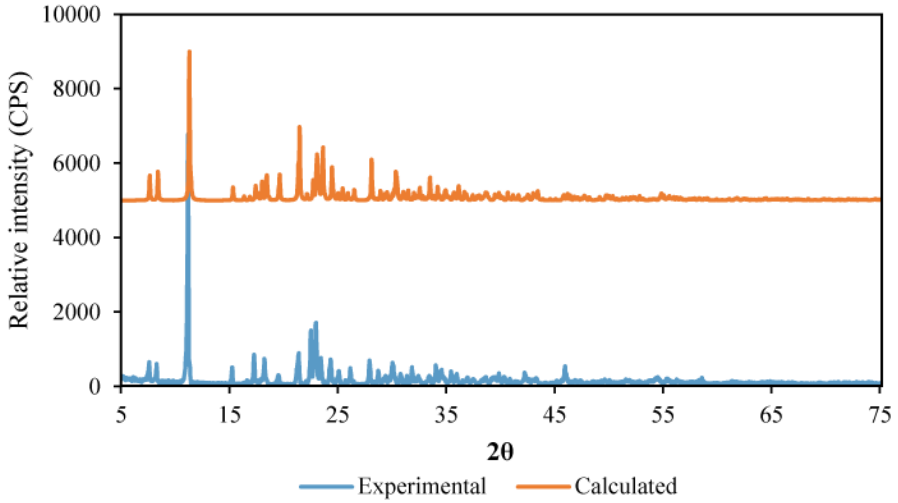

Figure S2. Powder X-ray diffraction pattern of the cocrystals **A1** (ACD)(*p*-DITFB), with the calculated diffraction pattern overlaid.

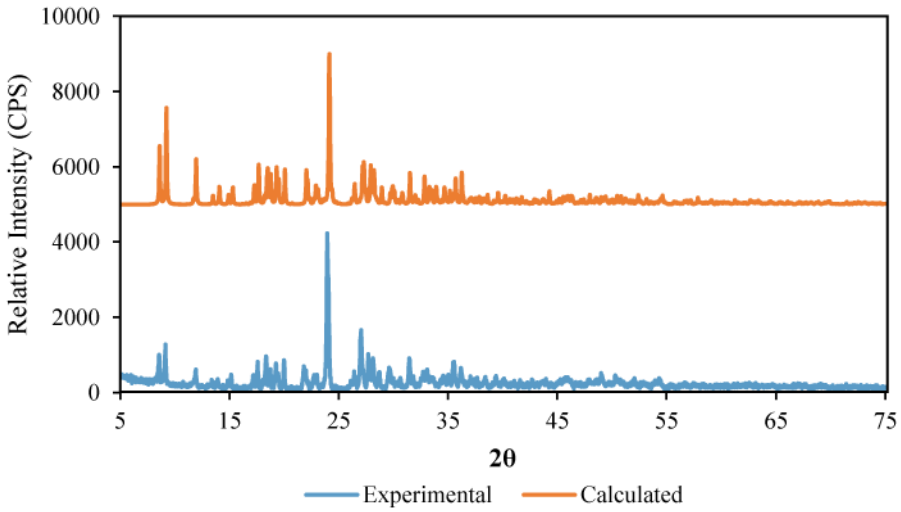

Figure S3. Powder X-ray diffraction pattern of the cocrystals **A2** (ACD)(*sym*-TFTIB), with the calculated diffraction pattern overlaid.

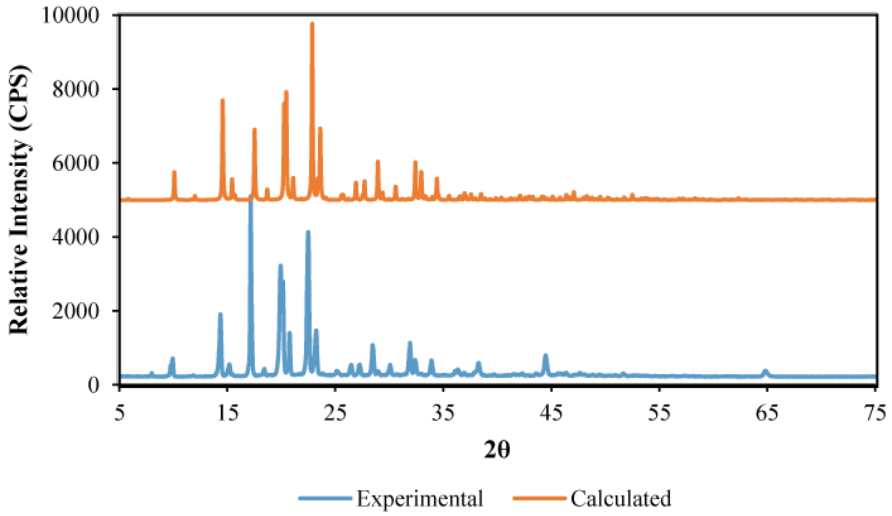

Figure S4. Powder X-ray diffraction pattern of **B** (1,10-phenanthroline, PHN), with the calculated diffraction pattern overlaid.

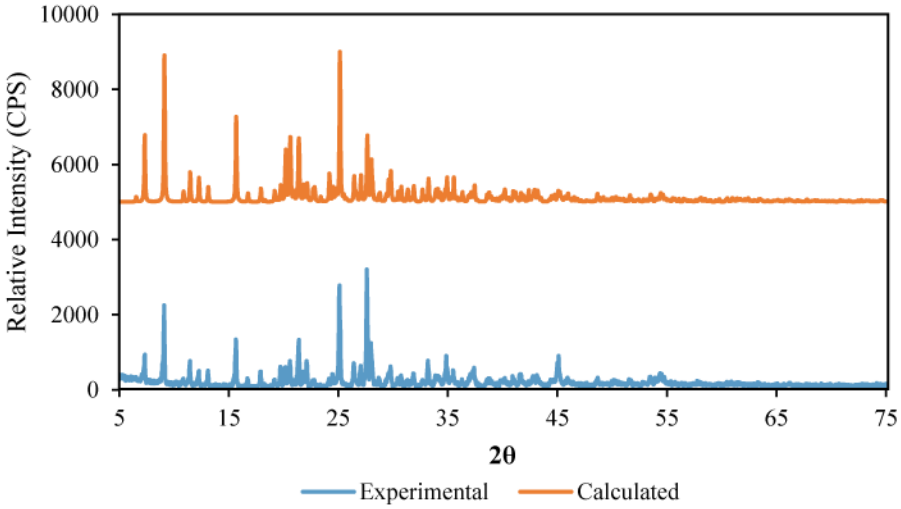

Figure S5. Powder X-ray diffraction pattern of the cocrystals **B1** (PHN)(*p*-DITFB), with the calculated diffraction pattern overlaid.

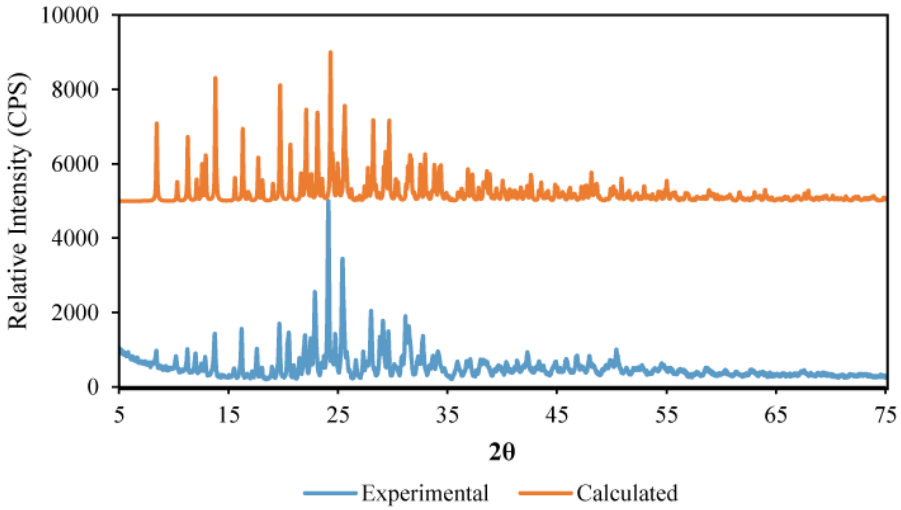

Figure S6. Powder X-ray diffraction pattern of the cocrystals **B2** (PHN)(*sym*-TFTIB), with the calculated diffraction pattern overlaid.

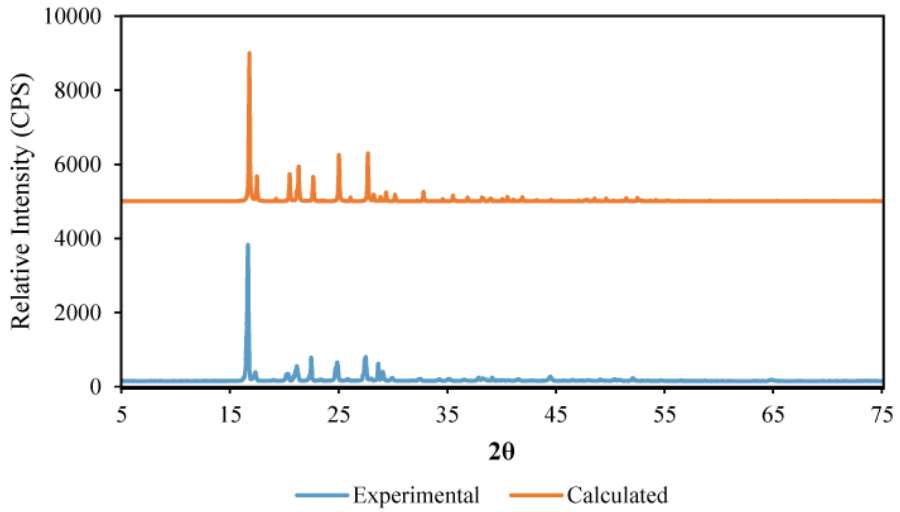

Figure S7. Powder X-ray diffraction pattern of **C** (2,3,5,6-tetramethylpyrazine, TMP), with the calculated diffraction pattern overlaid.

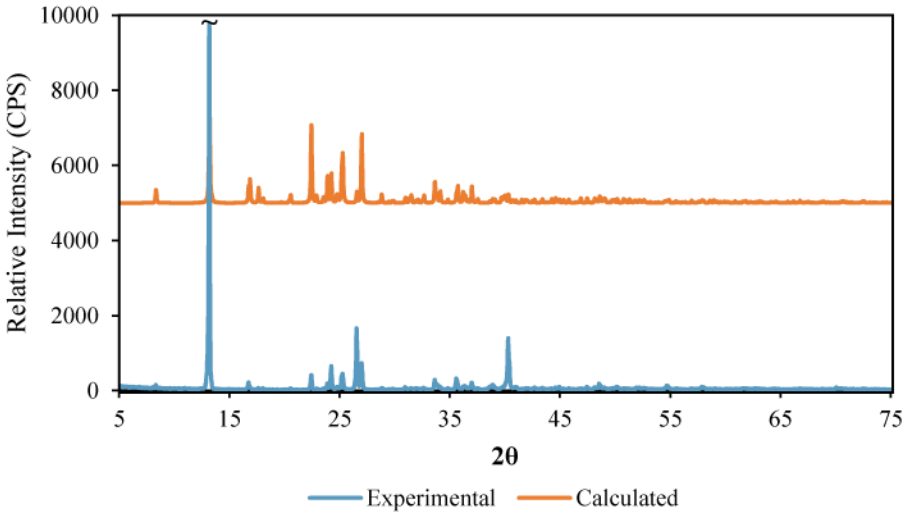

Figure S8. Powder X-ray diffraction pattern of the cocrystals **C1** (TMP)(*p*-DITFB), with the calculated diffraction pattern overlaid. The tilde at 13º indicates that it was cut for proper scaling.

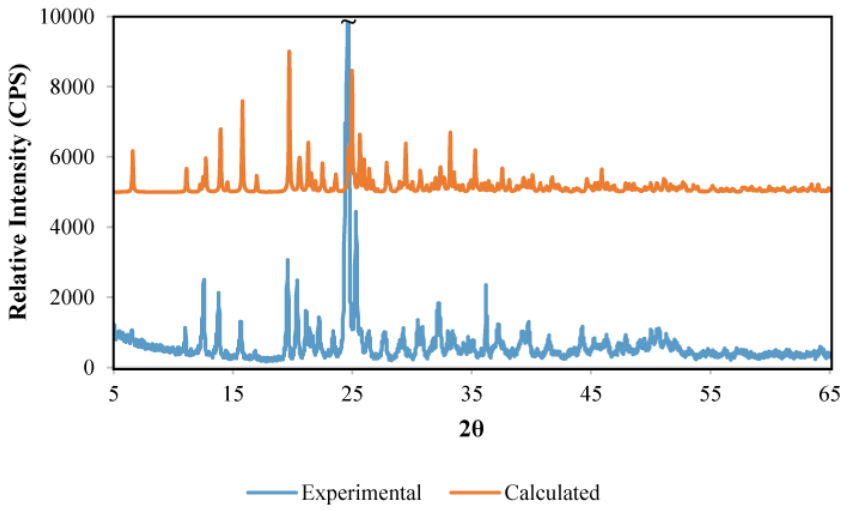

Figure S9. Powder X-ray diffraction pattern of the cocrystals **C2** (TMP)(*sym*-TFTIB), with the calculated diffraction pattern overlaid.

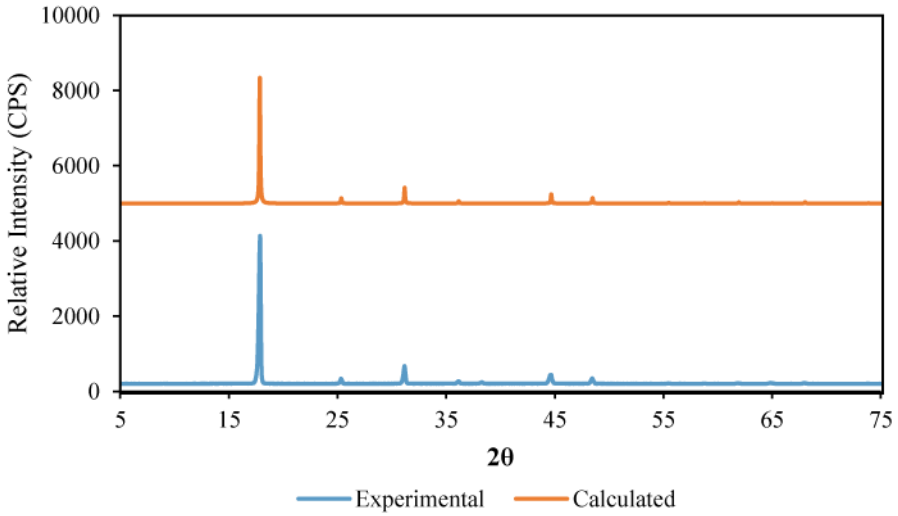

Figure S10. Powder X-ray diffraction pattern of **D** (urotropin, UTP), with the calculated diffraction pattern overlaid.

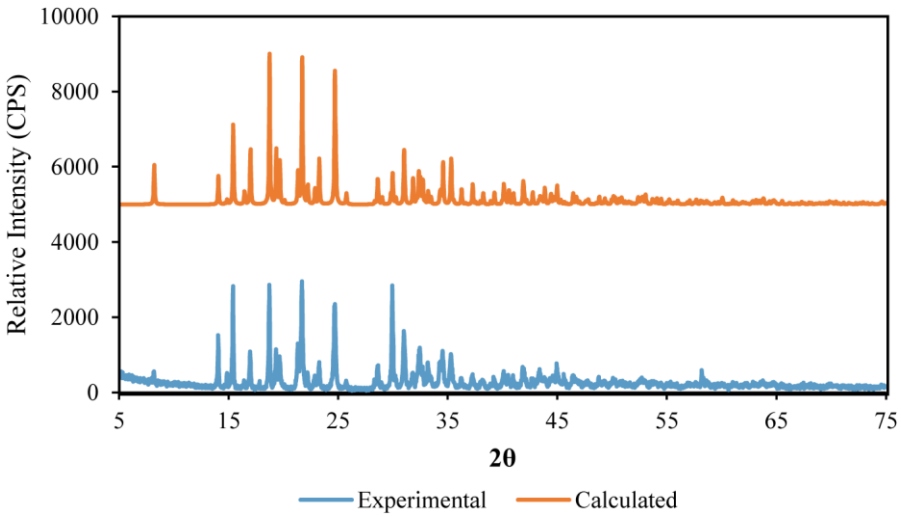

Figure S11. Powder X-ray diffraction pattern of the cocrystals **D1** (UTP)(*p*-DITFB), with the calculated diffraction pattern overlaid.

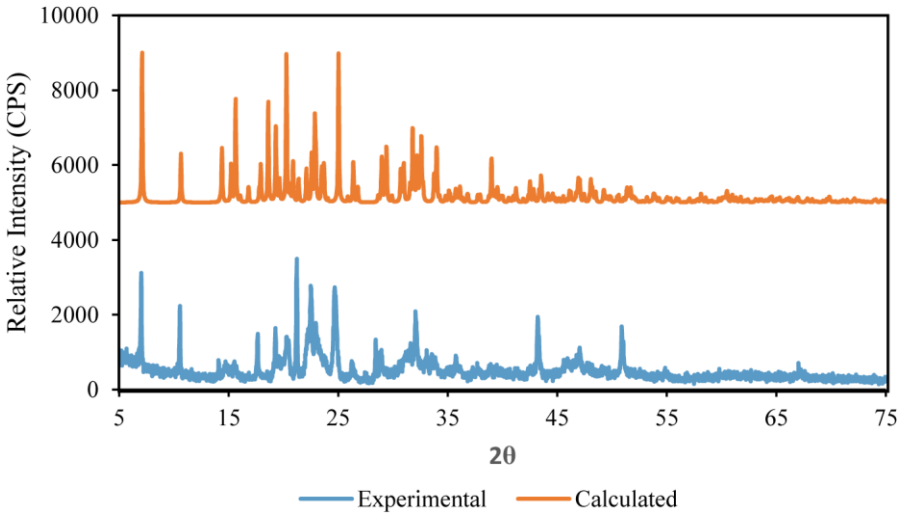

Figure S12. Powder X-ray diffraction pattern of the cocrystals **D2** (UTP)(*sym*-TFTIB), with the calculated diffraction pattern overlaid.

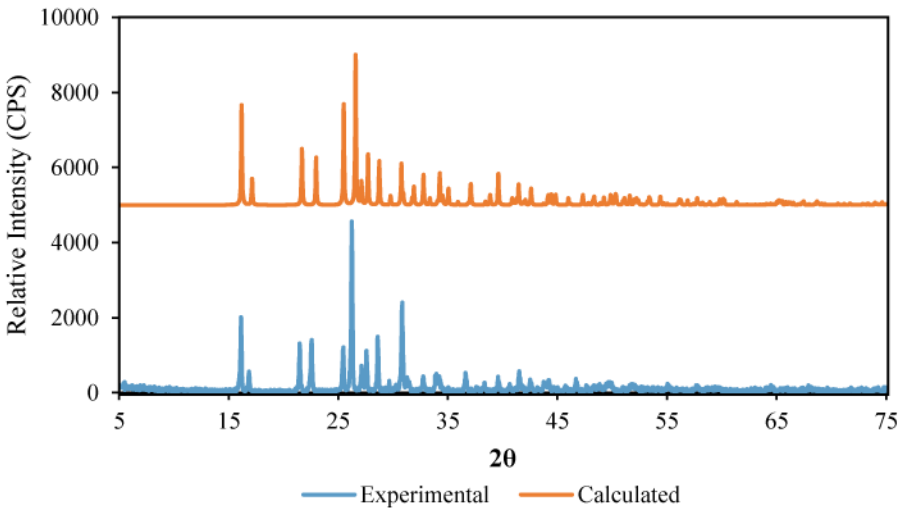

Figure 13. Powder X-ray diffraction pattern of the **1** (1,4-diiodotetrafluorobenzene, *p*-DITFB), with the calculated diffraction pattern overlaid.

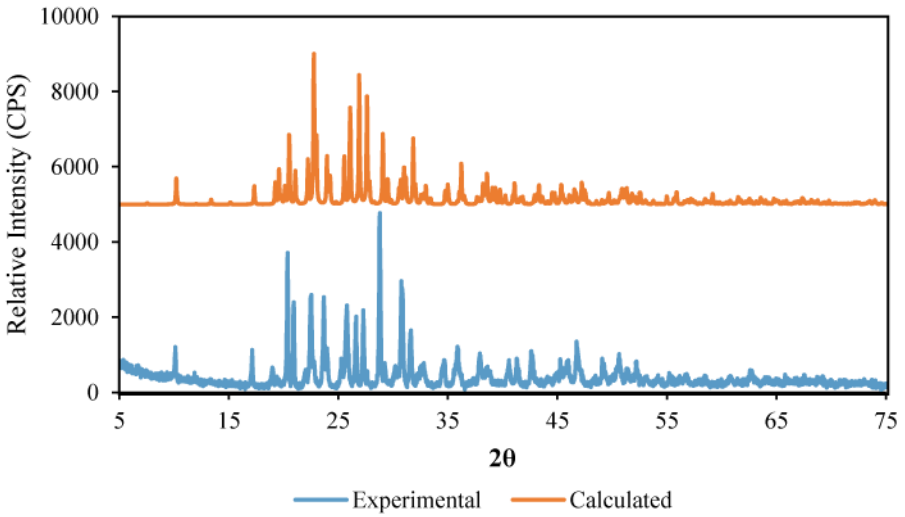

Figure 14. Powder X-ray diffraction pattern of **2** (1,3,5-trifluoro-2,4,6-triiodobenzene, *sym*-TFTIB), with the calculated diffraction pattern overlaid.

Table S1. Experimental powder X-ray diffraction conditions.

compound	2θ range	increment / º	rate / deg/min
1	5º to 75º	0.02	1.0
2	5º to 75º	0.02	1.0
A	5º to 75º	0.02	1.0
A1	5º to 75º	0.02	1.0
A2	5º to 75º	0.02	1.0
B	5º to 75º	0.02	1.0
B1	5º to 75º	0.02	1.0
B2	5º to 75º	0.02	0.1
C	5º to 75º	0.02	5.0
C1	5º to 75º	0.02	1.0
C2	5º to 65º	0.02	0.5
D	5º to 75º	0.02	5.0
D1	5º to 75º	0.02	1.0
D2	5º to 75º	0.02	1.0

SSNMR experimental details

Table S2. $^{13}C[^{1}H]$ CPMAS solid-state NMR experimental conditions.

compound	number of scans	recycle delay / s	MAS frequency / kHz
A	1024	60	10
A1	1024	58	12
A2	1024	60	12
B	1024	60	10
B1	1024	60	12
B2	1024	60	12
C	128	3	10
C1	4096	3	12
C2	7168	3	12
D	2400	5	10
D1	3072	5	12
D2	3072	5	12

Table S3. $^{13}C[^{19}F]$ CPMAS solid-state NMR experimental conditions.

compound	number of scans	recycle delay / s	MAS frequency / kHz
1	128	60	12
2	128	60	8
A1	1024	60	12
A2	256	60	8
B1	968	60	12
B2	168	60	8
C1	256	60	12
C2	1024	60	8
D1	128	60	12
D2	1024	60	8

Table S4. ^{19}F solid-state NMR experimental conditions.

compound	number of scans	recycle delay / s	MAS frequency / kHz
1	16	60	25
2	16	60	25
A1	16	60	25
A2	16	60	25
B1	16	60	25
B2	16	60	25
C1	16	60	25
C2	16	60	25
D1	16	60	25
D2	16	60	25

Computational details

Table S5. GIPAW-DFT calculation details for the unoptimized structures. The generalized gradient approximation (GGA) with the PBE functional was used for all compounds, with on-the-fly generated ultrasoft pseudopotentials.

compound	k-point set	energy cutoff (eV)
1	4x2x4	550
2	2x5x2	550
A	2x1x1	300
A1	2x4x1	550
A2	2x2x2	550
B	1x1x2	450
B1	5x2x1	550
B2	3x2x2	550
C	3x3x2	400
C1	2x4x2	550
C2	2x1x2	450
D	4x4x4	400
D1	4x1x4	550
D2	3x1x3	500

Table S6. GIPAW-DFT calculation details for the fully optimized structures. The generalized gradient approximation (GGA) with the PBE functional was used for all compounds, with on-the-fly generated ultrasoft pseudopotentials.

compound	k-point set	energy cutoff (eV)
1	4x2x4	550
2	2x5x2	550
A	4x1x2	400
A1	1x3x1	450
A2	2x2x1	500
B	1x1x2	500
B1	4x1x1	500
B2	2x1x1	500
C	3x3x2	400
C1	2x4x2	550
C2	2x1x2	450
D	4x4x4	400
D1	4x1x4	550
D2	3x1x3	500

Table S7. GIPAW-DFT calculation details for the unoptimized structures excluding the halogen bond donor. The generalized gradient approximation (GGA) with the PBE functional was used for all compounds, with on-the-fly generated ultrasoft pseudopotentials.

compound	k-point set	energy cutoff
A1	2x4x1	400 eV
A2	2x2x2	400 eV
B1	5x2x1	400 eV
B2	3x2x2	400 eV
C1	2x4x2	400 eV
C2	3x1x3	400 eV
D1	4x1x4	400 eV
D2	3x1x3	350 eV

Table S8. GIPAW-DFT calculation details for the fully optimized structure excluding the halogen bond donor. The generalized gradient approximation (GGA) with the PBE functional was used for all compounds, with on-the-fly generated ultrasoft pseudopotentials.

compound	k-point set	energy cutoff
A1	2x4x1	500 eV
A2	1x1x1	300 eV
B1	4x1x1	500 eV
B2	2x1x1	500 eV
C1	2x4x2	400 eV
C2	3x1x2	500 eV
D1	4x1x4	400 eV
D2	3x1x3	500 eV

Table S9. GIPAW-DFT calculation details for the unoptimized structure excluding the halogen bond acceptor. The generalized gradient approximation (GGA) with the PBE functional was used for all compounds, with on-the-fly generated ultrasoft pseudopotentials.

compound	k-point set	energy cutoff
A1	2x4x1	550 eV
A2	2x2x2	550 eV
B1	5x2x1	550 eV
B2	3x2x2	550 eV
C1	2x4x2	550 eV
C2	2x1x2	450 eV
D1	4x1x4	550 eV
D2	3x1x3	500 eV

Table S10. GIPAW-DFT calculation details for the fully optimized structure excluding the halogen bond acceptor. The generalized gradient approximation (GGA) with the PBE functional was used for all compounds, with on-the-fly generated ultrasoft pseudopotentials.

compound	k-point set	energy cutoff
A1	1x3x1	450 eV
A2	1x1x1	450 eV
B1	4x1x1	500 eV
B2	2x1x1	500 eV
C1	2x4x2	550 eV
C2	3x1x3	550 eV
D1	4x1x4	550 eV
D2	3x1x3	500 eV

Table S11. Experimental $\delta(^{13}C)$ chemical shifts and calculated $\sigma(^{13}C)$ magnetic shielding constants for each crystallographic site of the unoptimized and the optimized structure of compound **1**.

site label	experimental $\delta(^{13}C)$ / ppm	unoptimized $\sigma(^{13}C)$ / ppm	optimized $\sigma(^{13}C)$ / ppm
C1	147.6 ± 0.4	19.1	16.4
C2	147.6 ± 0.4	17.0	15.6
C3	76.8 ± 1.4	56.2	53.9

Table S12. Experimental $\delta(^{13}C)$ chemical shifts and calculated $\sigma(^{13}C)$ magnetic shielding constants for each crystallographic site of the unoptimized and the optimized structure of compound **2**.

site label	experimental $\delta(^{13}C)$ / ppm	unoptimized $\sigma(^{13}C)$ / ppm	optimized $\sigma(^{13}C)$ / ppm
C1	67.4 ± 2.4	62.9	59.5
C2	162.6 ± 0.9	7.3	4.8
C3	67.4 ± 2.4	62.0	58.1
C4	162.6 ± 0.9	4.4	3.4
C5	67.4 ± 2.4	59.1	56.1
C6	162.6 ± 0.9	6.7	4.2

Table S13. Experimental $\delta(^{13}C)$ chemical shifts and calculated $\sigma(^{13}C)$ magnetic shielding constants for each crystallographic site of the unoptimized and the optimized structure of compound **A**.

site label	experimental $\delta(^{13}C)$ / ppm	unoptimized $\sigma(^{13}C)$ / ppm	optimized $\sigma(^{13}C)$ / ppm
C1	126.4 ± 0.5[a]	50.7	44.8
C2	126.4 ± 0.5[a]	50.0	44.0
C3	148.7 ± 0.8	26.3	21.4
C4	136.9 ± 1.0	37.5	31.6
C5	148.7 ± 0.8	26.3	21.4
C6	128.7 ± 0.5[a]	41.8	36.4
C7	128.7 ± 0.5[a]	43.3	37.9
C8	128.7 ± 0.5[a]	45.6	40.8
C9	128.7 ± 0.5[a]	43.0	37.9
C10	123.9 ± 0.4[a]	51.6	45.4
C11	131.2 ± 0.4[a]	48.4	42.4
C12	131.2 ± 0.4[a]	45.7	39.5
C13	126.4 ± 0.5[a]	47.8	42.2
C14	148.7 ± 0.8	24.6	19.4
C15	148.7 ± 0.8	24.6	19.6
C16	126.4 ± 0.5[a]	50.0	43.8
C17	136.9 ± 1.0	35.8	29.6
C18	126.4 ± 0.5[a]	48.8	42.9
C19	128.7 ± 0.5[a]	45.0	39.1
C20	128.7 ± 0.5[a]	42.5	36.3
C21	128.7 ± 0.5[a]	40.5	35.0
C22	131.2 ± 0.4[a]	45.2	39.1
C23	128.7 ± 0.5[a]	44.5	38.9
C24	126.4 ± 0.5[a]	50.5	44.7
C25	126.4 ± 0.5[a]	49.0	42.8
C26	131.2 ± 0.4[a]	43.5	37.2

[a] Assignments are ambiguous as a result of the overlapping resonances.

Table S14. Experimental $\delta(^{13}C)$ chemical shifts and GIPAW-DFT calculated $\sigma(^{13}C)$ magnetic shielding constants for the unoptimized structure (unopt.), the optimized structure (opt.), the unoptimized structure with no donor (unopt. no donor), the optimized structure with no donor (opt. no donor), the unoptimized structure with no acceptor (unopt. no acc.), and the optimized structure with no acceptor (opt. no acc.) for compound **A1**.

site label	experimental $\delta(^{13}C)$ / ppm	unopt. $\sigma(^{13}C)$ / ppm	opt. $\sigma(^{13}C)$ / ppm	unopt. no donor $\sigma(^{13}C)$ / ppm	opt. no donor $\sigma(^{13}C)$ / ppm	unopt. no acc. $\sigma(^{13}C)$ / ppm	opt. no acc. $\sigma(^{13}C)$ / ppm
C1	138.1 ± 0.2[a]	40.4	28.3	41.9	31.2		
C2	148.7 ± 0.2	20.9	20.5	19.7	21.0		
C3	127.2 ± 0.2[a]	43.7	42.6	45.6	45.5		
C4	127.2 ± 0.2	48.1	37.3	47.3	39.3		
C5	127.2 ± 0.2[a]	48.9	39.7	52.6	44.3		
C6	130.9 ± 0.6[a]	42.9	35.0	46.2	40.3		
C7	127.2 ± 0.2[a]	44.8	37.2	44.3	37.6		
C8	148.7 ± 0.2	21.1	21.6	19.5	20.7		
C9	127.2 ± 0.2[a]	44.7	42.3	46.6	45.6		
C10	127.2 ± 0.2[a]	47.4	35.8	46.9	37.6		
C11	124.5 ± 0.2[a]	53.1	43.5	54.6	46.0		
C12	130.9 ± 0.6[a]	42.0	32.9	45.5	38.1		
C13	127.2 ± 0.2[a]	48.5	40.7	46.4	39.7		
C14	79.2 ± 2.3	54.9	50.7			58.4	58.0
C15	146.5 ± 0.4	20.2	17.3			18.4	16.2
C16	146.5 ± 0.4	20.0	17.9			18.5	16.1

[a] Assignments are ambiguous as a result of the overlapping resonances.

Table S15. Experimental $\delta(^{13}C)$ chemical shifts and GIPAW-DFT calculated $\sigma(^{13}C)$ magnetic shielding constants for the unoptimized structure (unopt.), the optimized structure (opt.), the unoptimized structure with no donor (unopt. no donor), the optimized structure with no donor (opt. no donor), the unoptimized structure with no acceptor (unopt. no acc.), and the optimized structure with no acceptor (opt. no acc.) for compound **A2**.

site label	experimental $\delta(^{13}C)$ / ppm	unopt. $\sigma(^{13}C)$ / ppm	opt. $\sigma(^{13}C)$ / ppm	unopt. no donor $\sigma(^{13}C)$ / ppm	opt. no donor $\sigma(^{13}C)$ / ppm	unopt. no acc. $\sigma(^{13}C)$ / ppm	opt. no acc. $\sigma(^{13}C)$ / ppm
C1	66.1 ± 4.7	63.4	56.1			66.8	61.7
C2	160.8 ± 0.8	9.1	6.5			7.5	5.1
C3	66.1 ± 4.7	67.8	62.9			69.0	64.2
C4	160.8 ± 0.8	8.9	6.3			6.3	3.3
C5	66.1 ± 4.7	62.9	57.3			62.8	56.6
C6	160.8 ± 0.8	8.8	6.0			6.6	3.4
C8	149.6 ± 0.3[a]	21.1	20.2	19.8	23.8		
C9	129.3 ± 0.2[a]	44.3	37.2	45.2	43.1		
C10	134.5 ± 0.2[a]	40.4	31.3	45.1	42.4		
C11	127.3 ± 0.2[a]	47.4	37.9	51.6	48.0		
C12	129.3 ± 0.2[a]	49.9	39.8	49.9	45.7		
C13	127.3 ± 0.2[a]	45.6	41.6	46.8	49.0		
C14	137.8 ± 0.1[a]	42.5	28.6	46.7	39.1		
C15	127.3 ± 0.2[a]	46.1	42.3	46.3	49.1		
C16	129.3 ± 0.2[a]	45.4	36.5	48.7	46.2		
C17	127.3 ± 0.2[a]	49.9	40.2	51.0	47.0		
C18	127.3 ± 0.2[a]	46.7	38.6	47.3	45.4		
C19	129.3 ± 0.2[a]	47.4	40.5	46.1	44.7		
C20	147.7 ± 0.2[a]	22.7	21.8	19.7	23.9		

[a] Assignments are ambiguous as a result of the overlapping resonances.

Table S16. Experimental δ(^{13}C) chemical shifts and calculated σ(^{13}C) magnetic shielding constants for each crystallographic site of the unoptimized and the optimized structure of compound **B**.

site label	experimental δ(^{13}C) / ppm	unoptimized σ(^{13}C) / ppm	optimized σ(^{13}C) / ppm
C1	150.7 ± 0.3	16.7	17.0
C2	122.2 ± 0.1	44.5	43.5
C3	145.0 ± 0.2	24.8	23.5
C4	127.8 ± 0.2[a]	40.6	39.5
C5	134.8 ± 0.1	35.2	33.4
C6	127.8 ± 0.2[a]	39.8	38.1
C7	145.0 ± 0.2	24.6	24.2
C8	127.8 ± 0.2[a]	40.2	39.7
C9	127.8 ± 0.2[a]	38.0	38.5
C10	137.7 ± 0.2[a]	31.7	29.2
C11	122.2 ± 0.1	48.1	46.4
C12	150.7 ± 0.3	16.2	16.8
C13	150.7 ± 0.3	16.9	16.0
C14	122.2 ± 0.1	46.9	46.1
C15	145.0 ± 0.2	23.6	23.4
C16	127.8 ± 0.2[a]	41.0	41.2
C17	134.8 ± 0.1[a]	33.4	32.4
C18	129.0 ± 0.3[a]	37.8	37.1
C19	145.0 ± 0.2	24.6	23.6
C20	127.8 ± 0.2[a]	40.6	38.6
C21	127.8 ± 0.2[a]	41.1	39.8
C22	137.7 ± 0.2[a]	32.0	28.4
C23	122.2 ± 0.1	46.5	45.8
C24	150.7 ± 0.3	14.5	15.8
C25	150.7 ± 0.3	16.2	15.5

C26	122.2 ± 0.1	48.7	46.4
C27	145.0 ± 0.2	23.9	23.3
C28	127.8 ± 0.2[a]	40.9	41.1
C29	134.8 ± 0.1[a]	34.0	33.8
C30	127.8 ± 0.2[a]	39.6	38.0
C31	145.0 ± 0.2	24.6	24.0
C32	127.8 ± 0.2[a]	40.5	39.2
C33	127.8 ± 0.2[a]	40.8	40.1
C34	137.7 ± 0.2[a]	30.4	28.7
C35	122.2 ± 0.1	45.4	45.7
C36	150.7 ± 0.3	16.9	16.5

[a] Assignments are ambiguous.

Table S17. Experimental $\delta(^{13}C)$ chemical shifts and GIPAW-DFT calculated $\sigma(^{13}C)$ magnetic shielding constants for the unoptimized structure (unopt.), the optimized structure (opt.), the unoptimized structure with no donor (unopt. no donor), the optimized structure with no donor (opt. no donor), the unoptimized structure with no acceptor (unopt. no acc.), and the optimized structure with no acceptor (opt. no acc.) for compound **B1**.

site label	experimental $\delta(^{13}C)$ / ppm	unopt. $\sigma(^{13}C)$ / ppm	opt. $\sigma(^{13}C)$ / ppm	unopt. no donor $\sigma(^{13}C)$ / ppm	opt. no donor $\sigma(^{13}C)$ / ppm	unopt. no acc. $\sigma(^{13}C)$ / ppm	opt. no acc. $\sigma(^{13}C)$ / ppm
C1	144.0 ± 0.3	23.3	25.3	20.6	23.5		
C2	150.0 ± 0.2	26.6	17.6	26.4	19.3		
C3	120.6 ± 0.2	59.2	47.4	61.6	50.2		
C4	134.4 ± 0.2	47.2	32.9	50.2	37.6		
C5	127.3 ± 0.2[a]	46.2	40.4	46.9	43.0		
C6	125.9 ± 0.2[a]	53.3	40.5	54.2	42.9		
C7	125.9 ± 0.2[a]	53.9	37.8	56.8	43.1		
C8	127.3 ± 0.2[a]	44.8	41.2	46.4	43.9		
C9	132.6 ± 0.2	47.8	34.3	50.7	38.9		
C10	120.6 ± 0.2	59.9	46.8	62.3	50.4		
C11	148.4 ± 0.2	29.5	18.9	27.4	18.6		
C12	144.0 ± 0.3	24.8	24.7	22.8	23.1		
C13	79.1 ± 1.9	53.9	48.0			59.0	56.9
C14	147.7 ± 0.5[a]	22.5	16.5			22.0	16.4
C15	147.7 ± 0.5[a]	19.2	15.8			19.1	16.6
C16	76.7 ± 1.8	58.4	51.9			59.1	55.5
C17	145.9 ± 0.4[a]	24.4	18.5			23.3	16.7
C18	145.9 ± 0.4[a]	24.0	17.9			23.0	16.9

[a] Assignments are ambiguous as a result of the overlapping resonances.

Table S18. Experimental $\delta(^{13}C)$ chemical shifts and GIPAW-DFT calculated $\sigma(^{13}C)$ magnetic shielding constants for the unoptimized structure (unopt.), the optimized structure (opt.), the unoptimized structure with no donor (unopt. no donor), the optimized structure with no donor (opt. no donor), the unoptimized structure with no acceptor (unopt. no acc.), and the optimized structure with no acceptor (opt. no acc.) for compound **B2**.

site label	experimental $\delta(^{13}C)$ / ppm	unopt. $\sigma(^{13}C)$ / ppm	opt. $\sigma(^{13}C)$ / ppm	unopt. no donor $\sigma(^{13}C)$ / ppm	opt. no donor $\sigma(^{13}C)$ / ppm	unopt. no acc. $\sigma(^{13}C)$ / ppm	opt. no acc. $\sigma(^{13}C)$ / ppm
C1	68.5 ± 3.3	63.4	56.1			66.8	61.7
C2	162.3 ± 1.4	9.1	6.5			7.5	5.1
C3	68.5 ± 3.3	67.8	62.9			69.0	64.2
C4	162.3 ± 1.4	8.9	6.3			6.3	3.3
C5	68.5 ± 3.3	62.9	57.3			62.8	56.6
C6	162.3 ± 1.4	8.8	6.0			6.6	3.4
C8	149.4 ± 0.2	21.1	20.2	25.7	23.5		
C9	124.5 ± 0.3[a]	44.3	37.2	57.9	19.3		
C10	136.5 ± 0.2	40.4	31.3	44.6	50.2		
C11	128.6 ± 0.3[a]	47.4	37.9	45.1	37.6		
C12	128.6 ± 0.3[a]	49.9	39.8	48.9	43.0		
C13	128.6 ± 0.3[a]	45.6	41.6	50.4	42.9		
C14	128.6 ± 0.3[a]	42.5	28.6	44.6	43.1		
C15	136.5 ± 0.2	46.1	42.3	42.7	43.9		
C16	124.5 ± 0.3[a]	45.4	36.5	55.5	38.9		
C17	151.4 ± 0.2	49.9	40.2	23.7	50.4		
C19	145.3 ± 0.5	46.7	38.6	21.6	18.6		
C20	145.3 ± 0.5	47.4	40.5	22.0	23.1		

[a] Assignments are ambiguous as a result of the overlapping resonances.

Table S19. Experimental $\delta(^{13}C)$ chemical shifts and calculated $\sigma(^{13}C)$ magnetic shielding constants for each crystallographic site of the unoptimized and the optimized structure of compound **C**.

site label	experimental $\delta(^{13}C)$ / ppm	unoptimized $\sigma(^{13}C)$ / ppm	optimized $\sigma(^{13}C)$ / ppm
C1	149.7 ± 0.1	14.4	15.0
C2	149.0 ± 0.1	15.3	16.2
C3	21.7 ± 0.1	153.3	150.6
C4	21.1 ± 0.1	154.1	151.6

Table S20. Experimental $\delta(^{13}C)$ chemical shifts and GIPAW-DFT calculated $\sigma(^{13}C)$ magnetic shielding constants for the unoptimized structure (unopt.), the optimized structure (opt.), the unoptimized structure with no donor (unopt. no donor), the optimized structure with no donor (opt. no donor), the unoptimized structure with no acceptor (unopt. no acc.), and the optimized structure with no acceptor (opt. no acc.) for compound **C1**.

site label	experimental $\delta(^{13}C)$ / ppm	unopt. $\sigma(^{13}C)$ / ppm	opt. $\sigma(^{13}C)$ / ppm	unopt. no donor $\sigma(^{13}C)$ / ppm	opt. no donor $\sigma(^{13}C)$ / ppm	unopt. no acc. $\sigma(^{13}C)$ / ppm	opt. no acc. $\sigma(^{13}C)$ / ppm
C1	80.3 ± 2.4	57.0	51.0			60.8	58.4
C2	147.4 ± 0.4	20.3	16.1			19.3	15.7
C3	147.4 ± 0.4	20.1	16.3			18.6	15.6
C4	149.4 ± 0.2	15.2	14.4	18.4	17.6		
C5	149.4 ± 0.2	17.2	15.2	19.1	17.0		
C6	22.4 ± 0.2	172.6	149.2	176.1	152.2		
C7	22.4 ± 0.2	172.9	148.9	174.7	150.6		

Table S21. Experimental $\delta(^{13}C)$ chemical shifts and GIPAW-DFT calculated $\sigma(^{13}C)$ magnetic shielding constants for the unoptimized structure (unopt.), the optimized structure (opt.), the unoptimized structure with no donor (unopt. no donor), the optimized structure with no donor (opt. no donor), the unoptimized structure with no acceptor (unopt. no acc.), and the optimized structure with no acceptor (opt. no acc.) for compound **C2**.

site label	experimental $\delta(^{13}C)$ / ppm	unopt. $\sigma(^{13}C)$ / ppm	opt. $\sigma(^{13}C)$ / ppm	unopt. no donor $\sigma(^{13}C)$ / ppm	opt. no donor $\sigma(^{13}C)$ / ppm	unopt. no acc. $\sigma(^{13}C)$ / ppm	opt. no acc. $\sigma(^{13}C)$ / ppm
C1	71.5 ± 11.0	56.5	50.2			58.7	58.5
C2	162.3 ± 0.8	5.3	3.6			3.7	3.6
C3	71.5 ± 11.0	68.3	62.5			59.0	59.2
C4	162.3 ± 0.8	7.8	5.2			3.2	3.3
C5	71.5 ± 11.0	62.2	55.6			62.9	62.9
C6	162.3 ± 0.8	6.6	3.3			4.6	4.6
C7	22.7 ± 0.1	168.7	149.3	172.1	152.5		
C8	149.7 ± 0.3	15.7	14.0	18.8	19.4		
C9	149.7 ± 0.3	17.3	14.7	20.3	19.4		
C10	22.7 ± 0.1	170.1	149.7	173.1	152.4		
C11	22.7 ± 0.1	169.4	149.6	171.6	151.9		
C12	149.7 ± 0.3	16.9	14.9	18.7	18.9		
C13	149.7 ± 0.3	16.0	14.0	19.4	18.9		
C14	22.7 ± 0.1	168.7	148.6	172.2	152.1		

Table S22. Experimental $\delta(^{13}C)$ chemical shifts and calculated $\sigma(^{13}C)$ magnetic shielding constants for each crystallographic site of the unoptimized and the optimized structure of compound **D**.

site label	experimental $\delta(^{13}C)$ / ppm	unoptimized $\sigma(^{13}C)$ / ppm	optimized $\sigma(^{13}C)$ / ppm
C1	73.4 ± 0.1	100.0	95.3
	73.2 ± 0.1	100.0	95.3

Table S23. Experimental $\delta(^{13}C)$ chemical shifts and GIPAW-DFT calculated $\sigma(^{13}C)$ magnetic shielding constants for the unoptimized structure (unopt.), the optimized structure (opt.), the unoptimized structure with no donor (unopt. no donor), the optimized structure with no donor (opt. no donor), the unoptimized structure with no acceptor (unopt. no acc.), and the optimized structure with no acceptor (opt. no acc.) for compound **D1**.

site label	experimental $\delta(^{13}C)$ / ppm	unopt. $\sigma(^{13}C)$ / ppm	opt. $\sigma(^{13}C)$ / ppm	unopt. no donor $\sigma(^{13}C)$ / ppm	opt. no donor $\sigma(^{13}C)$ / ppm	unopt. no acc. $\sigma(^{13}C)$ / ppm	opt. no acc. $\sigma(^{13}C)$ / ppm
C1	74.7 ± 0.2[a]	112.0	93.9	110.8	91.7		
C2	71.8 ± 0.2[a]	111.8	94.5	110.7	92.7		
C3	74.7 ± 0.2[a]	112.0	93.9	110.8	91.7		
C4	71.8 ± 0.2[a]	111.8	94.5	110.7	92.7		
C5	80.8 ± 2.7	52.6	48.3			57.4	57.0
C6	147.1 ± 0.4	19.5	16.5			18.3	15.5
C7	147.1 ± 0.4	20.4	16.7			19.4	16.0

[a] Assignments are ambiguous.

Table S24. Experimental $\delta(^{13}C)$ chemical shifts and GIPAW-DFT calculated $\sigma(^{13}C)$ magnetic shielding constants for the unoptimized structure (unopt.), the optimized structure (opt.), the unoptimized structure with no donor (unopt. no donor), the optimized structure with no donor (opt. no donor), the unoptimized structure with no acceptor (unopt. no acc.), and the optimized structure with no acceptor (opt. no acc.) for compound **D2**.

site label	experimental $\delta(^{13}C)$ / ppm	unopt. $\sigma(^{13}C)$ / ppm	opt. $\sigma(^{13}C)$ / ppm	unopt. no donor $\sigma(^{13}C)$ / ppm	opt. no donor $\sigma(^{13}C)$ / ppm	unopt. no acc. $\sigma(^{13}C)$ / ppm	opt. no acc. $\sigma(^{13}C)$ / ppm
C1	71.8 ± 7.9	57.8	52.8			62.1	60.5
C2	162.8 ± 0.9	5.5	3.9			5.4	4.8
C3	71.8 ± 7.9	64.3	59.3			62.2	57.0
C4	162.8 ± 0.9	4.7	3.8			3.9	3.4
C5	71.8 ± 7.9	58.2	54.0			61.3	59.7
C6	162.8 ± 0.9	5.9	2.3			7.3	3.9
C7	74.9 ± 0.4[a]	112.9	93.8	113.0	93.4		
C8	74.9 ± 0.4[a]	112.6	94.2	113.8	95.0		
C9	71.8 ± 0.2[a]	113.2	94.5	113.6	94.6		
C10	74.9 ± 0.4[a]	110.3	92.3	112.1	93.0		

[a] Assignments are ambiguous.

^{19}F Solid-State NMR Calculation Results

Table S25. Experimental $\delta(^{19}F)$ chemical shifts and GIPAW-DFT calculated $\sigma(^{19}F)$ magnetic shielding constants for each crystallographic site of the unoptimized and the optimized structure of compound **1**.

site label	experimental $\delta(^{19}F)$ / ppm	unoptimized $\sigma(^{19}F)$ / ppm	optimized $\sigma(^{19}F)$ / ppm
F1	-115.6 ± 0.3	259.7	258.2
F2	-112.5 ± 0.4	255.8	253.8

Table S26. Experimental $\delta(^{19}F)$ chemical shifts and GIPAW-DFT calculated $\sigma(^{19}F)$ magnetic shielding constants for each crystallographic site of the unoptimized and the optimized structure of compound **2**.

site label	experimental $\delta(^{19}F)$ / ppm	unoptimized $\sigma(^{19}F)$ / ppm	optimized $\sigma(^{19}F)$ / ppm
F1	-66.5 ± 0.3	201.3	207.3
F2	-64.2 ± 0.3	202.6	202.5
F3	-61.9 ± 0.2	194.8	198.3

Table S27. Experimental $\delta(^{19}F)$ chemical shifts and GIPAW-DFT calculated $\sigma(^{19}F)$ magnetic shielding constants for each crystallographic site of the unoptimized structure, the optimized structure, the unoptimized structure with no acceptor (unopt. no acceptor), and the optimized structure with no acceptor (opt. no acceptor) for compound **A1**.

site label	experimental $\delta(^{19}F)$ / ppm	unoptimized $\sigma(^{19}F)$ / ppm	optimized $\sigma(^{19}F)$ / ppm	unopt. no acceptor $\sigma(^{19}F)$ / ppm	opt. no acceptor $\sigma(^{19}F)$ / ppm
F1	-114.1 ± 0.7	264.9	260.8	261.9	266.8
F2	-114.1 ± 0.7	264.4	258.8	260.2	261.7

Table S28. Experimental $\delta(^{19}F)$ chemical shifts and GIPAW-DFT calculated $\sigma(^{19}F)$ magnetic shielding constants for each crystallographic site of the unoptimized structure, the optimized structure, the unoptimized structure with no acceptor (unopt. no acceptor), and the optimized structure with no acceptor (opt. no acceptor) for compound **A2**.

site label	experimental $\delta(^{19}F)$ / ppm	unoptimized $\sigma(^{19}F)$ / ppm	optimized $\sigma(^{19}F)$ / ppm	unopt. no acceptor $\sigma(^{19}F)$ / ppm	opt. no acceptor $\sigma(^{19}F)$ / ppm
F2	-72.3 ± 0.4	216.1	216.7	205.1	210.1
F4	-70.8 ± 0.3	212.5	211.7	203.5	206.4
F6	-68.3 ± 0.3	211.9	212.2	199.6	204.3

Table S29. Experimental $\delta(^{19}F)$ chemical shifts and GIPAW-DFT calculated $\sigma(^{19}F)$ magnetic shielding constants for each crystallographic site of the unoptimized structure, the optimized structure, the unoptimized structure with no acceptor (unopt. no acceptor), and the optimized structure with no acceptor (opt. no acceptor) for compound **B1**.

site label	experimental $\delta(^{19}F)$ / ppm	unoptimized $\sigma(^{19}F)$ / ppm	optimized $\sigma(^{19}F)$ / ppm	unopt. no acceptor $\sigma(^{19}F)$ / ppm	opt. no acceptor $\sigma(^{19}F)$ / ppm
F1	-118.3 ± 0.4	273.3	264.9	267.9	263.8
F2	-115.0 ± 0.3	269.7	259.4	261.9	257.6
F3	-118.3 ± 0.4	271.1	263.9	272.4	266.0
F4	-114.9 ± 0.3	264.8	261.9	264.9	263.8

Table S30. Experimental $\delta(^{19}F)$ chemical shifts and GIPAW-DFT calculated $\sigma(^{19}F)$ magnetic shielding constants for each crystallographic site of the unoptimized structure, the optimized structure, the unoptimized structure with no acceptor (unopt. no acceptor), and the optimized structure with no acceptor (opt. no acceptor) for compound **B2**.

site label	experimental $\delta(^{19}F)$ / ppm	unoptimized $\sigma(^{19}F)$ / ppm	optimized $\sigma(^{19}F)$ / ppm	unopt. no acceptor $\sigma(^{19}F)$ / ppm	opt. no acceptor $\sigma(^{19}F)$ / ppm
F2	-71.6 ± 0.3	215.5	212.5	202.5	210.1
F4	-71.6 ± 0.3	215.2	217.4	205.1	204.5
F6	-71.6 ± 0.3	215.5	214.4	207.2	208.5

Table S31. Experimental $\delta(^{19}F)$ chemical shifts and GIPAW-DFT calculated $\sigma(^{19}F)$ magnetic shielding constants for each crystallographic site of the unoptimized structure, the optimized structure, the unoptimized structure with no acceptor (unopt. no acceptor), and the optimized structure with no acceptor (opt. no acceptor) for compound **C1**.

site label	experimental $\delta(^{19}F)$ / ppm	unoptimized $\sigma(^{19}F)$ / ppm	optimized $\sigma(^{19}F)$ / ppm	unopt. no acceptor $\sigma(^{19}F)$ / ppm	opt. no acceptor $\sigma(^{19}F)$ / ppm
F1	-119.2 ± 0.5	272.2	264.5	266.3	261.6
F2	-119.2 ± 0.5	270.1	263.4	263.5	261.6

Table S32. Experimental $\delta(^{19}F)$ chemical shifts and GIPAW-DFT calculated $\sigma(^{19}F)$ magnetic shielding constants for each crystallographic site of the unoptimized structure, the optimized structure, the unoptimized structure with no acceptor (unopt. no acceptor), and the optimized structure with no acceptor (opt. no acceptor) for compound **C2**.

site label	experimental $\delta(^{19}F)$ / ppm	unoptimized $\sigma(^{19}F)$ / ppm	optimized $\sigma(^{19}F)$ / ppm	unopt. no acceptor $\sigma(^{19}F)$ / ppm	opt. no acceptor $\sigma(^{19}F)$ / ppm
F1	-72.3 ± 0.4	220.9	219.4	213.9	211.0
F2	-68.5 ± 0.3	212.5	211.4	207.1	204.0
F3	-72.3 ± 0.4	218.9	217.5	209.0	204.4

Table S33. Experimental $\delta(^{19}F)$ chemical shifts and GIPAW-DFT calculated $\sigma(^{19}F)$ magnetic shielding constants for each crystallographic site of the unoptimized structure, the optimized structure, the unoptimized structure with no acceptor (unopt. no acceptor), and the optimized structure with no acceptor (opt. no acceptor) for compound **D1**.

site label	experimental $\delta(^{19}F)$ / ppm	unoptimized $\sigma(^{19}F)$ / ppm	optimized $\sigma(^{19}F)$ / ppm	unopt. no acceptor $\sigma(^{19}F)$ / ppm	opt. no acceptor $\sigma(^{19}F)$ / ppm
F1	-120.4 ± 0.3	273.5	265.3	267.9	262.4
F2	-117.4 ± 0.3	269.3	263.0	258.0	260.3

Table S34. Experimental $\delta(^{19}F)$ chemical shifts and GIPAW-DFT calculated $\sigma(^{19}F)$ magnetic shielding constants for each crystallographic site of the unoptimized structure, the optimized structure, the unoptimized structure with no acceptor (unopt. no acceptor), and the optimized structure with no acceptor (opt. no acceptor) for compound **D2**.

site label	experimental $\delta(^{19}F)$ / ppm	unoptimized $\sigma(^{19}F)$ / ppm	optimized $\sigma(^{19}F)$ / ppm	unopt. no acceptor $\sigma(^{19}F)$ / ppm	opt. no acceptor $\sigma(^{19}F)$ / ppm
F1	-77.4 ± 0.3	220.8	221.0	201.4	209.5
F2	-72.4 ± 0.4	217.7	217.9	201.4	208.3
F3	-70.4 ± 0.4	213.9	212.5	201.1	206.5

Fractional Coordinates of the Geometry Optimized Structures

All lattice parameters were fixed during the geometry optimizations. The resulting lattice parameters, cell angles, and geometry optimized fractional coordinates are reported for each compound.

Compound **1 -** (*p*-DITFB)

Lattice parameters(A)		Cell Angles	
a =	6.218700	alpha =	90.000000
b =	11.616800	beta =	93.610001
c =	5.787600	gamma =	90.000000

Cell Contents

Element	Atom Number	Fractional coordinates of atoms u	v	w
C	1	0.419536	0.400431	0.395072
C	2	0.307724	0.454136	0.566153
C	3	0.613616	0.445493	0.327498
C	4	0.580470	0.900432	0.104931
C	5	0.692272	0.954134	0.933837
C	6	0.386392	0.945495	0.172509
C	7	0.580464	0.599569	0.604928
C	8	0.692276	0.545864	0.433847
C	9	0.386384	0.554507	0.672502
C	10	0.419530	0.099568	0.895069
C	11	0.307728	0.045866	0.066163
C	12	0.613608	0.054505	0.827491
F	1	0.121597	0.407054	0.627058
F	2	0.335615	0.304623	0.295212
F	3	0.878390	0.907050	0.872905
F	4	0.664393	0.804627	0.204804
F	5	0.878403	0.592946	0.372942
F	6	0.664385	0.695377	0.704788
F	7	0.121610	0.092950	0.127095
F	8	0.335607	0.195373	0.795196
I	1	0.781210	0.363151	0.072132
I	2	0.218794	0.863154	0.427871
I	3	0.218791	0.636849	0.927868
I	4	0.781206	0.136846	0.572129

Compound **2** – (*sym*-TFTIB)

Lattice parameters(A)		Cell Angles	
a =	13.818000	alpha =	90.000000
b =	4.758000	beta =	107.080002
c =	15.385000	gamma =	90.000000

Cell Contents

Element	Atom Number	Fractional coordinates of atoms u	v	w
C	1	0.025819	0.730472	0.710606
C	2	0.957628	0.674156	0.625706
C	3	0.876496	0.489984	0.615552
C	4	0.864995	0.362342	0.693554
C	5	0.931256	0.413527	0.779853
C	6	0.011597	0.597099	0.786530
C	7	0.474181	0.230476	0.789397
C	8	0.542370	0.174158	0.874292
C	9	0.623506	0.989984	0.884450
C	10	0.635004	0.862342	0.806444
C	11	0.568745	0.913525	0.720147
C	12	0.488403	0.097097	0.713469
C	13	0.974182	0.269527	0.289397
C	14	0.042371	0.325843	0.374292
C	15	0.123504	0.510015	0.384448
C	16	0.135004	0.637659	0.306444
C	17	0.068744	0.586472	0.220149
C	18	0.988403	0.402903	0.213469
C	19	0.525820	0.769524	0.210604
C	20	0.457629	0.825842	0.125707
C	21	0.376495	0.010016	0.115551
C	22	0.364995	0.137659	0.193555
C	23	0.431256	0.086474	0.279853
C	24	0.511596	0.902903	0.286531
F	1	0.970509	0.800493	0.551808
F	2	0.788285	0.181173	0.685290
F	3	0.079172	0.641476	0.868509
F	4	0.529491	0.300494	0.948191
F	5	0.711715	0.681171	0.814710
F	6	0.420828	0.141475	0.631491
F	7	0.029491	0.199506	0.448192
F	8	0.211714	0.818827	0.314710
F	9	0.920829	0.358524	0.131492
F	10	0.470509	0.699506	0.051809
F	11	0.288285	0.318829	0.185290
F	12	0.579172	0.858526	0.368509
I	1	0.149110	0.007241	0.724850
I	2	0.774699	0.415025	0.486676
I	3	0.910368	0.217811	0.895159
I	4	0.350889	0.507241	0.775150
I	5	0.725300	0.915026	0.013324
I	6	0.589632	0.717811	0.604842

```
x  I            7          0.850890   0.992759   0.275150   x
x  I            8          0.225301   0.584975   0.513325   x
x  I            9          0.089632   0.782189   0.104841   x
x  I           10          0.649111   0.492759   0.224850   x
x  I           11          0.274700   0.084973   0.986676   x
x  I           12          0.410368   0.282189   0.395158   x
xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
```

Compound **A** – (ACD)

Lattice parameters(A)		Cell Angles	
a =	6.069300	alpha =	90.000000
b =	18.818100	beta =	95.154999
c =	16.283001	gamma =	90.000000

Element	Atom Number	Fractional coordinates of atoms u	v	w
H	1	0.634242	0.405008	0.864812
H	2	0.444492	0.541881	0.931830
H	3	0.396261	0.318023	0.053249
H	4	0.671243	0.524287	0.797633
H	5	0.617441	0.285634	0.930292
H	6	0.900165	0.630357	0.774546
H	7	0.285101	0.639056	0.841935
H	8	0.185556	0.208815	0.082948
H	9	0.800601	0.191991	0.022556
H	10	0.153520	0.022354	0.210592
H	11	0.779817	0.235096	0.184798
H	12	0.939616	0.020669	0.059665
H	13	0.074702	0.138150	0.276553
H	14	0.855731	0.893578	0.025505
H	15	0.250643	0.907070	0.144655
H	16	0.191336	0.261231	0.313770
H	17	0.514293	0.837215	0.068104
H	18	0.540305	0.310050	0.267144
H	19	0.365759	0.904913	0.635204
H	20	0.555474	0.041745	0.568194
H	21	0.603654	0.817869	0.446787
H	22	0.328765	0.024291	0.702372
H	23	0.382509	0.785538	0.569737
H	24	0.099837	0.130285	0.725487
H	25	0.714808	0.139003	0.658087
H	26	0.814459	0.708833	0.416991
H	27	0.199427	0.691961	0.477415
H	28	0.846313	0.522217	0.289394
H	29	0.220289	0.735142	0.315222
H	30	0.060288	0.520573	0.440344
H	31	0.925400	0.638204	0.223461
H	32	0.144314	0.393493	0.474467
H	33	0.749420	0.407117	0.355339
H	34	0.808693	0.761144	0.186198
H	35	0.485739	0.337169	0.431868
H	36	0.459634	0.810001	0.232823
H	37	0.365758	0.594992	0.135188
H	38	0.555508	0.458119	0.068170
H	39	0.603738	0.681977	0.946751
H	40	0.328757	0.475713	0.202367
H	41	0.382559	0.714366	0.069708
H	42	0.099834	0.369643	0.225454
H	43	0.714899	0.360944	0.158065
H	44	0.814444	0.791185	0.917052
H	45	0.199399	0.808009	0.977444
H	46	0.846480	0.977646	0.789409

x	H	47	0.220183	0.764904	0.815202	x
x	H	48	0.060384	0.979332	0.940335	x
x	H	49	0.925298	0.861850	0.723447	x
x	H	50	0.144268	0.106422	0.974495	x
x	H	51	0.749357	0.092930	0.855345	x
x	H	52	0.808664	0.738769	0.686230	x
x	H	53	0.485707	0.162785	0.931896	x
x	H	54	0.459695	0.689950	0.732856	x
x	H	55	0.634242	0.095087	0.364796	x
x	H	56	0.444526	0.958255	0.431806	x
x	H	57	0.396346	0.182131	0.553214	x
x	H	58	0.671235	0.975709	0.297629	x
x	H	59	0.617492	0.214462	0.430263	x
x	H	60	0.900162	0.869715	0.274513	x
x	H	61	0.285192	0.860997	0.341913	x
x	H	62	0.185540	0.291167	0.583009	x
x	H	63	0.800573	0.308039	0.522585	x
x	H	64	0.153687	0.477783	0.710606	x
x	H	65	0.779711	0.264858	0.684778	x
x	H	66	0.939712	0.479427	0.559656	x
x	H	67	0.074600	0.361796	0.776539	x
x	H	68	0.855686	0.606507	0.525533	x
x	H	69	0.250580	0.592883	0.644661	x
x	H	70	0.191307	0.238856	0.813802	x
x	H	71	0.514261	0.662831	0.568132	x
x	H	72	0.540366	0.189999	0.767177	x
x	C	1	0.928431	0.470674	0.875550	x
x	C	2	0.902880	0.355096	0.939581	x
x	C	3	0.152936	0.475195	0.913367	x
x	C	4	0.806215	0.409719	0.890510	x
x	C	5	0.128328	0.364639	0.974666	x
x	C	6	0.278649	0.537507	0.899998	x
x	C	7	0.227033	0.309952	0.026309	x
x	C	8	0.841328	0.527863	0.825258	x
x	C	9	0.787923	0.291604	0.957041	x
x	C	10	0.968564	0.586538	0.812663	x
x	C	11	0.188245	0.591260	0.850755	x
x	C	12	0.110042	0.249771	0.042136	x
x	C	13	0.888527	0.240170	0.007195	x
x	C	14	0.645369	0.036644	0.122326	x
x	C	15	0.565383	0.143423	0.183889	x
x	C	16	0.361717	0.115553	0.210742	x
x	C	17	0.305787	0.045112	0.190871	x
x	C	18	0.446136	0.003756	0.146856	x
x	C	19	0.625365	0.214823	0.205205	x
x	C	20	0.790393	0.994995	0.077777	x
x	C	21	0.228320	0.159788	0.257157	x
x	C	22	0.743300	0.925117	0.059469	x
x	C	23	0.402432	0.931150	0.126276	x
x	C	24	0.292817	0.228016	0.277059	x
x	C	25	0.547775	0.892735	0.083926	x
x	C	26	0.492807	0.255612	0.250582	x
x	C	27	0.071641	0.970645	0.624441	x
x	C	28	0.097123	0.855061	0.560413	x
x	C	29	0.847132	0.975165	0.586631	x
x	C	30	0.193813	0.909676	0.609490	x
x	C	31	0.871659	0.864606	0.525332	x

x	C	32	0.721359	0.037458	0.600007	x
x	C	33	0.772953	0.809908	0.473700	x
x	C	34	0.158691	0.027840	0.674731	x
x	C	35	0.212073	0.791562	0.542958	x
x	C	36	0.031404	0.086502	0.687331	x
x	C	37	0.811710	0.091221	0.649248	x
x	C	38	0.890013	0.749756	0.457834	x
x	C	39	0.111512	0.740145	0.492773	x
x	C	40	0.354583	0.536621	0.377692	x
x	C	41	0.434632	0.643400	0.316128	x
x	C	42	0.638311	0.615520	0.289266	x
x	C	43	0.694172	0.545069	0.309128	x
x	C	44	0.553805	0.503739	0.353160	x
x	C	45	0.374668	0.714807	0.294810	x
x	C	46	0.209577	0.494947	0.422229	x
x	C	47	0.771696	0.659766	0.242857	x
x	C	48	0.256716	0.425066	0.440522	x
x	C	49	0.597569	0.431139	0.373730	x
x	C	50	0.707162	0.727980	0.222933	x
x	C	51	0.452264	0.392697	0.416067	x
x	C	52	0.507191	0.755580	0.249405	x
x	C	53	0.071569	0.529326	0.124450	x
x	C	54	0.097120	0.644904	0.060419	x
x	C	55	0.847064	0.524805	0.086633	x
x	C	56	0.193785	0.590281	0.109490	x
x	C	57	0.871672	0.635361	0.025334	x
x	C	58	0.721351	0.462493	0.100002	x
x	C	59	0.772967	0.690048	0.973691	x
x	C	60	0.158672	0.472137	0.174742	x
x	C	61	0.212077	0.708396	0.042959	x
x	C	62	0.031436	0.413462	0.187337	x
x	C	63	0.811755	0.408740	0.149245	x
x	C	64	0.889958	0.750229	0.957864	x
x	C	65	0.111473	0.759830	0.992805	x
x	C	66	0.354631	0.963356	0.877674	x
x	C	67	0.434617	0.856577	0.816111	x
x	C	68	0.638283	0.884447	0.789258	x
x	C	69	0.694213	0.954888	0.809129	x
x	C	70	0.553864	0.996244	0.853144	x
x	C	71	0.374635	0.785177	0.794795	x
x	C	72	0.209607	0.005005	0.922223	x
x	C	73	0.771680	0.840212	0.742843	x
x	C	74	0.256700	0.074883	0.940531	x
x	C	75	0.597568	0.068850	0.873724	x
x	C	76	0.707183	0.771984	0.722941	x
x	C	77	0.452225	0.107265	0.916074	x
x	C	78	0.507193	0.744388	0.749418	x
x	C	79	0.928359	0.029355	0.375559	x
x	C	80	0.902877	0.144939	0.439587	x
x	C	81	0.152869	0.024835	0.413369	x
x	C	82	0.806187	0.090324	0.390510	x
x	C	83	0.128341	0.135394	0.474668	x
x	C	84	0.278641	0.962542	0.399992	x
x	C	85	0.227047	0.190092	0.526300	x
x	C	86	0.841309	0.972160	0.325269	x
x	C	87	0.787927	0.208438	0.457042	x
x	C	88	0.968596	0.913498	0.312669	x

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x  C           89         0.188290   0.908779   0.350752   x
x  C           90         0.109987   0.250244   0.542166   x
x  C           91         0.888488   0.259855   0.507227   x
x  C           92         0.645417   0.463379   0.622308   x
x  C           93         0.565368   0.356600   0.683872   x
x  C           94         0.361689   0.384480   0.710734   x
x  C           95         0.305828   0.454931   0.690872   x
x  C           96         0.446195   0.496261   0.646840   x
x  C           97         0.625332   0.285193   0.705190   x
x  C           98         0.790423   0.505053   0.577771   x
x  C           99         0.228305   0.340234   0.757143   x
x  C          100         0.743284   0.574934   0.559478   x
x  C          101         0.402431   0.568862   0.626270   x
x  C          102         0.292839   0.272020   0.777067   x
x  C          103         0.547736   0.607303   0.583933   x
x  C          104         0.492809   0.244420   0.750595   x
x  N            1         0.247796   0.423250   0.961538   x
x  N            2         0.701221   0.104597   0.140341   x
x  N            3         0.752226   0.923219   0.538472   x
x  N            4         0.298765   0.604578   0.359671   x
x  N            5         0.752204   0.576750   0.038462   x
x  N            6         0.298779   0.895403   0.859659   x
x  N            7         0.247774   0.076781   0.461529   x
x  N            8         0.701235   0.395422   0.640329   x
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Compound **A1** – (ACD)(*p*-DITFB)

Lattice parameters(A)		Cell Angles	
a =	10.490700	alpha =	90.000000
b =	5.567900	beta =	90.764999
c =	23.078699	gamma =	90.000000

Cell Contents

Element	Atom Number	Fractional coordinates of atoms u	v	w
H	1	0.039757	0.146900	0.279528
H	2	0.205723	0.170708	0.203117
H	3	0.388270	0.386033	0.160513
H	4	0.466228	0.770404	0.204837
H	5	0.363379	0.936245	0.292058
H	6	0.874947	0.137731	0.355892
H	7	0.780248	0.319380	0.443196
H	8	0.870747	0.701161	0.484184
H	9	0.054047	0.900233	0.437799
H	10	0.960243	0.646899	0.220472
H	11	0.794277	0.670707	0.296883
H	12	0.611730	0.886033	0.339487
H	13	0.533772	0.270404	0.295163
H	14	0.636621	0.436244	0.207942
H	15	0.125053	0.637731	0.144108
H	16	0.219752	0.819380	0.056804
H	17	0.129253	0.201160	0.015816
H	18	0.945953	0.400233	0.062201
H	19	0.960243	0.853101	0.720472
H	20	0.794277	0.829292	0.796883
H	21	0.611730	0.613966	0.839487
H	22	0.533772	0.229595	0.795163
H	23	0.636621	0.063755	0.707942
H	24	0.125053	0.862269	0.644108
H	25	0.219752	0.680620	0.556804
H	26	0.129253	0.298839	0.515816
H	27	0.945953	0.099767	0.562201
H	28	0.039757	0.353101	0.779528
H	29	0.205723	0.329292	0.703117
H	30	0.388270	0.113967	0.660513
H	31	0.466228	0.729596	0.704837
H	32	0.363379	0.563756	0.792058
H	33	0.874947	0.362269	0.855892
H	34	0.780248	0.180620	0.943196
H	35	0.870747	0.798839	0.984184
H	36	0.054047	0.599767	0.937799
C	1	0.075838	0.315001	0.297706
C	2	0.225249	0.649798	0.298345
C	3	0.179374	0.429458	0.272238
C	4	0.240747	0.337770	0.222252

x	C	5	0.342016	0.457821	0.198777	x
x	C	6	0.386334	0.675759	0.224131	x
x	C	7	0.329927	0.769317	0.272489	x
x	C	8	0.071356	0.633513	0.370138	x
x	C	9	0.018869	0.413502	0.346589	x
x	C	10	0.913062	0.304065	0.374041	x
x	C	11	0.860981	0.406024	0.422394	x
x	C	12	0.912498	0.622706	0.445547	x
x	C	13	0.014471	0.733964	0.420264	x
x	C	14	0.573312	0.837911	0.034411	x
x	C	15	0.569446	0.819883	0.974254	x
x	C	16	0.501836	0.020140	0.059498	x
x	C	17	0.924162	0.815001	0.202294	x
x	C	18	0.774752	0.149799	0.201655	x
x	C	19	0.820626	0.929458	0.227762	x
x	C	20	0.759253	0.837770	0.277748	x
x	C	21	0.657985	0.957822	0.301223	x
x	C	22	0.613666	0.175759	0.275869	x
x	C	23	0.670073	0.269318	0.227511	x
x	C	24	0.928644	0.133514	0.129862	x
x	C	25	0.981132	0.913502	0.153412	x
x	C	26	0.086938	0.804065	0.125959	x
x	C	27	0.139019	0.906024	0.077607	x
x	C	28	0.087501	0.122706	0.054454	x
x	C	29	0.985529	0.233964	0.079736	x
x	C	30	0.426688	0.337911	0.465589	x
x	C	31	0.430554	0.319882	0.525746	x
x	C	32	0.498164	0.520141	0.440502	x
x	C	33	0.924162	0.685000	0.702294	x
x	C	34	0.774751	0.350202	0.701655	x
x	C	35	0.820626	0.570543	0.727762	x
x	C	36	0.759253	0.662230	0.777748	x
x	C	37	0.657984	0.542178	0.801223	x
x	C	38	0.613666	0.324241	0.775869	x
x	C	39	0.670073	0.230683	0.727511	x
x	C	40	0.928644	0.366487	0.629861	x
x	C	41	0.981131	0.586498	0.653411	x
x	C	42	0.086938	0.695936	0.625958	x
x	C	43	0.139019	0.593976	0.577606	x
x	C	44	0.087502	0.377294	0.554453	x
x	C	45	0.985529	0.266036	0.579736	x
x	C	46	0.426688	0.162089	0.965589	x
x	C	47	0.430554	0.180117	0.025746	x
x	C	48	0.498164	0.979860	0.940502	x
x	C	49	0.075838	0.184999	0.797705	x
x	C	50	0.225248	0.850201	0.798345	x
x	C	51	0.179374	0.070542	0.772238	x
x	C	52	0.240747	0.162230	0.722252	x
x	C	53	0.342015	0.042178	0.698776	x
x	C	54	0.386334	0.824241	0.724131	x
x	C	55	0.329927	0.730682	0.772489	x
x	C	56	0.071355	0.866486	0.870138	x
x	C	57	0.018868	0.086498	0.846588	x
x	C	58	0.913062	0.195935	0.874041	x
x	C	59	0.860981	0.093976	0.922393	x
x	C	60	0.912498	0.877294	0.945546	x
x	C	61	0.014471	0.766036	0.920264	x

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x  C          62         0.573312   0.662089   0.534411   x
x  C          63         0.569446   0.680117   0.474254   x
x  C          64         0.501836   0.479859   0.559498   x
x  N           1         0.172234   0.744830   0.346208   x
x  N           2         0.827766   0.244830   0.153792   x
x  N           3         0.827765   0.255170   0.653791   x
x  N           4         0.172234   0.755169   0.846208   x
x  F           1         0.634800   0.643695   0.947268   x
x  F           2         0.500250   0.044812   0.117702   x
x  F           3         0.365201   0.143695   0.552732   x
x  F           4         0.499749   0.544813   0.382298   x
x  F           5         0.365201   0.356304   0.052732   x
x  F           6         0.499750   0.955189   0.882298   x
x  F           7         0.634799   0.856305   0.447268   x
x  F           8         0.500251   0.455188   0.617702   x
x  I           1         0.684658   0.597427   0.085920   x
x  I           2         0.315342   0.097426   0.414080   x
x  I           3         0.315342   0.402573   0.914080   x
x  I           4         0.684658   0.902574   0.585920   x
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Compound **A2** – (ACD)(*sym*-TFTIB)

Lattice parameters(A)		Cell Angles	
a =	10.507900	alpha =	90.000000
b =	12.563200	beta =	102.489998
c =	15.156300	gamma =	90.000000

Cell Contents

Element	Atom Number	Fractional coordinates of atoms u	v	w
H	1	0.829011	0.829656	0.324516
H	2	0.603457	0.528730	0.190520
H	3	1.080398	0.855666	0.080918
H	4	0.964896	0.694193	0.008249
H	5	0.997943	0.970869	0.330495
H	6	0.563593	0.387939	0.073408
H	7	0.845517	0.530479	-0.059296
H	8	1.122443	0.983577	0.208188
H	9	0.683905	0.387968	-0.051288
H	10	0.171072	0.329963	0.175498
H	11	0.396476	0.028537	0.309459
H	12	-0.080357	0.355898	0.419088
H	13	0.035218	0.194596	0.491792
H	14	0.002040	0.470799	0.169493
H	15	0.436425	-0.112029	0.426596
H	16	0.154436	0.030382	0.559286
H	17	-0.122542	0.483459	0.291803
H	18	0.316101	-0.111998	0.551302
H	19	0.170989	0.170345	0.675485
H	20	0.396543	0.471270	0.809480
H	21	-0.080398	0.144334	0.919082
H	22	0.035104	0.305806	0.991751
H	23	0.002057	0.029131	0.669505
H	24	0.436407	0.612061	0.926592
H	25	0.154483	0.469521	1.059296
H	26	-0.122443	0.016423	0.791812
H	27	0.316095	0.612032	1.051288
H	28	0.828928	0.670037	0.824502
H	29	0.603524	0.971463	0.690541
H	30	1.080357	0.644102	0.580912
H	31	0.964783	0.805404	0.508208
H	32	0.997960	0.529201	0.830507
H	33	0.563575	1.112029	0.573404
H	34	0.845564	0.969618	0.440714
H	35	1.122541	0.516541	0.708197
H	36	0.683899	1.111998	0.448698
C	1	0.554882	0.610074	0.627713
C	2	0.664733	0.585878	0.502113
C	3	0.726952	0.496948	0.546807
C	4	0.860820	0.759676	0.201317
C	5	0.621126	0.521420	0.670014
C	6	0.705623	0.462427	0.629807

x	C	7	0.578198	0.640146	0.543983	x
x	C	8	0.933140	0.767577	0.130600	x
x	C	9	0.749829	0.609574	0.135280	x
x	C	10	0.885774	0.835889	0.272498	x
x	C	11	0.656560	0.527905	0.136334	x
x	C	12	0.818890	0.610489	0.062307	x
x	C	13	1.026905	0.850219	0.134816	x
x	C	14	0.910118	0.691265	0.061832	x
x	C	15	0.978508	0.913590	0.275028	x
x	C	16	0.634916	0.450289	0.071019	x
x	C	17	0.792803	0.528955	-0.004605	x
x	C	18	1.049960	0.921096	0.205576	x
x	C	19	0.703701	0.450303	-0.000141	x
x	C	20	0.445025	0.109798	0.872110	x
x	C	21	0.335185	0.085848	0.997824	x
x	C	22	0.272881	-0.003089	0.953210	x
x	C	23	0.139198	0.259676	0.298658	x
x	C	24	0.378942	0.020935	0.830018	x
x	C	25	0.294238	-0.037724	0.870272	x
x	C	26	0.421702	0.139986	0.955846	x
x	C	27	0.066888	0.267600	0.369385	x
x	C	28	0.250145	0.109555	0.364715	x
x	C	29	0.114270	0.335932	0.227508	x
x	C	30	0.343391	0.027859	0.363654	x
x	C	31	0.181095	0.110499	0.437709	x
x	C	32	-0.026885	0.350235	0.365189	x
x	C	33	0.089940	0.191348	0.438189	x
x	C	34	0.021479	0.413573	0.224978	x
x	C	35	0.365072	-0.049717	0.428992	x
x	C	36	0.207167	0.028939	0.504603	x
x	C	37	-0.049996	0.421051	0.294403	x
x	C	38	0.296289	-0.049695	0.500142	x
x	C	39	0.445118	0.389926	0.372287	x
x	C	40	0.335267	0.414122	0.497886	x
x	C	41	0.273048	0.503052	0.453193	x
x	C	42	0.139180	0.240324	0.798683	x
x	C	43	0.378874	0.478580	0.329986	x
x	C	44	0.294377	0.537573	0.370193	x
x	C	45	0.421801	0.359854	0.456017	x
x	C	46	0.066860	0.232423	0.869400	x
x	C	47	0.250170	0.390426	0.864720	x
x	C	48	0.114226	0.164112	0.727502	x
x	C	49	0.343440	0.472095	0.863666	x
x	C	50	0.181110	0.389511	0.937693	x
x	C	51	-0.026905	0.149781	0.865184	x
x	C	52	0.089882	0.308735	0.938168	x
x	C	53	0.021493	0.086410	0.724972	x
x	C	54	0.365084	0.549711	0.928981	x
x	C	55	0.207197	0.471045	1.004605	x
x	C	56	-0.049959	0.078904	0.794424	x
x	C	57	0.296299	0.549697	1.000141	x
x	C	58	0.554975	0.890201	0.127891	x
x	C	59	0.664815	0.914152	0.002177	x
x	C	60	0.727119	1.003089	0.046790	x
x	C	61	0.860802	0.740323	0.701342	x
x	C	62	0.621058	0.979065	0.169982	x
x	C	63	0.705762	1.037724	0.129728	x

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x  C           64         0.578298   0.860014   0.044154   x
x  C           65         0.933112   0.732400   0.630615   x
x  C           66         0.749855   0.890445   0.635285   x
x  C           67         0.885730   0.664068   0.772492   x
x  C           68         0.656609   0.972141   0.636346   x
x  C           69         0.818905   0.889501   0.562291   x
x  C           70         1.026886   0.649765   0.634811   x
x  C           71         0.910060   0.808652   0.561811   x
x  C           72         0.978521   0.586427   0.775021   x
x  C           73         0.634928   1.049717   0.571008   x
x  C           74         0.792834   0.971061   0.495396   x
x  C           75         1.049996   0.578949   0.705597   x
x  C           76         0.703711   1.049695   0.499858   x
x  N            1         0.772308   0.682180   0.202714   x
x  N            2         0.227700   0.182167   0.297281   x
x  N            3         0.227692   0.317820   0.797286   x
x  N            4         0.772300   0.817833   0.702719   x
x  F            1         0.514833   0.726028   0.502299   x
x  F            2         0.604766   0.492644   0.752571   x
x  F            3         0.811699   0.442105   0.508855   x
x  F            4         0.485261   0.225780   0.997550   x
x  F            5         0.395759  -0.009024   0.747829   x
x  F            6         0.188249  -0.057993   0.991219   x
x  F            7         0.485166   0.273971   0.497701   x
x  F            8         0.395234   0.507356   0.247429   x
x  F            9         0.188300   0.557895   0.491145   x
x  F           10         0.514739   0.774219   0.002450   x
x  F           11         0.604241   1.009024   0.252171   x
x  F           12         0.811751   1.057993   0.008781   x
x  I            1         0.701720   0.634443   0.375550   x
x  I            2         0.426445   0.696381   0.689904   x
x  I            3         0.799369   0.326133   0.692301   x
x  I            4         0.298278   0.134482   1.124400   x
x  I            5         0.573471   0.196232   0.810005   x
x  I            6         0.200522  -0.174007   0.807771   x
x  I            7         0.298279   0.365557   0.624450   x
x  I            8         0.573554   0.303619   0.310096   x
x  I            9         0.200631   0.673867   0.307699   x
x  I           10         0.701722   0.865518  -0.124399   x
x  I           11         0.426529   0.803768   0.189995   x
x  I           12         0.799477   1.174007   0.192229   x
xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
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Compound **B** - (PHN)

Lattice parameters(A)		Cell Angles	
a =	17.521601	alpha =	90.000000
b =	17.521601	beta =	90.000000
c =	8.433700	gamma =	120.000000

Cell Contents

Element	Atom Number	Fractional coordinates of atoms u	v	w
H	1	0.201855	0.655176	0.548115
H	2	0.074776	0.649207	0.697377
H	3	0.925813	0.577222	0.567013
H	4	0.831925	0.499040	0.333575
H	5	0.818087	0.436740	0.064348
H	6	0.887878	0.412645	0.829190
H	7	0.025010	0.432113	0.695725
H	8	0.169065	0.514094	0.841232
H	9	0.888768	0.035116	0.489552
H	10	0.765923	0.999475	0.681252
H	11	0.611718	0.886890	0.601818
H	12	0.508432	0.786437	0.392951
H	13	0.486920	0.718103	0.127569
H	14	0.549724	0.706714	0.869023
H	15	0.682703	0.757837	0.693913
H	16	0.830036	0.875967	0.795297
H	17	0.808269	0.360533	0.462459
H	18	0.916547	0.343065	0.292987
H	19	0.980127	0.252879	0.397568
H	20	0.991574	0.163822	0.620584
H	21	0.944713	0.098221	0.887867
H	22	0.856002	0.076398	0.132364
H	23	0.756310	0.113150	0.288072
H	24	0.710518	0.215706	0.165762
H	25	0.326639	0.677710	0.321411
H	26	0.235347	0.625256	0.239655
H	27	0.902702	0.966814	0.082059
H	28	0.986491	0.992203	0.981236
H	29	0.669475	0.325358	0.977592
H	30	0.729850	0.300870	0.881148
H	31	0.344815	0.546671	0.214795
H	32	0.350799	0.425570	0.364060
H	33	0.422780	0.348590	0.233681
H	34	0.500945	0.332879	1.000250
H	35	0.563249	0.381343	0.731025
H	36	0.587372	0.475242	0.495886
H	37	0.567885	0.592890	0.362395
H	38	0.485857	0.654923	0.507853
H	39	0.964862	0.853625	0.156218
H	40	0.000540	0.766455	0.347943

x	H	41	0.113119	0.724835	0.268498	x
x	H	42	0.213560	0.721995	0.059632	x
x	H	43	0.281921	0.768845	0.794270	x
x	H	44	0.293288	0.843018	0.535699	x
x	H	45	0.242125	0.924833	0.360567	x
x	H	46	0.123976	0.954004	0.461940	x
x	H	47	0.639455	0.447732	0.129144	x
x	H	48	0.656942	0.573477	0.959660	x
x	H	49	0.747143	0.727244	0.064228	x
x	H	50	0.836170	0.827749	0.287268	x
x	H	51	0.901735	0.846488	0.554584	x
x	H	52	0.923519	0.779611	0.799104	x
x	H	53	0.886838	0.643172	0.954775	x
x	H	54	0.784383	0.494817	0.832397	x
x	H	55	0.322321	0.648987	0.988182	x
x	H	56	0.374732	0.610155	0.906244	x
x	H	57	0.033087	0.935856	0.748800	x
x	H	58	0.007898	0.994409	0.647970	x
x	H	59	0.674558	0.344127	0.644348	x
x	H	60	0.699263	0.429043	0.547887	x
x	H	61	0.453338	0.798139	0.881447	x
x	H	62	0.574434	0.925233	0.030731	x
x	H	63	0.651411	0.074192	0.900354	x
x	H	64	0.667126	0.168073	0.666913	x
x	H	65	0.618671	0.181911	0.397692	x
x	H	66	0.524764	0.112122	0.162536	x
x	H	67	0.407099	0.974988	0.029074	x
x	H	68	0.345061	0.830931	0.174545	x
x	H	69	0.146350	0.111231	0.822883	x
x	H	70	0.233553	0.234082	0.014599	x
x	H	71	0.275182	0.388281	0.935155	x
x	H	72	0.278007	0.491565	0.726301	x
x	H	73	0.231141	0.513076	0.460954	x
x	H	74	0.156984	0.450273	0.202362	x
x	H	75	0.075162	0.317297	0.027241	x
x	H	76	0.045991	0.169973	0.128610	x
x	H	77	0.552269	0.191707	0.795821	x
x	H	78	0.426524	0.083465	0.626317	x
x	H	79	0.272755	0.019912	0.730867	x
x	H	80	0.172251	0.008420	0.953914	x
x	H	81	0.153503	0.055257	0.221209	x
x	H	82	0.220388	0.143954	0.465732	x
x	H	83	0.356838	0.243679	0.621419	x
x	H	84	0.505182	0.289472	0.499099	x
x	H	85	0.350982	0.673362	0.654778	x
x	H	86	0.389953	0.764648	0.572973	x
x	H	87	0.064154	0.097318	0.415355	x
x	H	88	0.005621	0.013508	0.314664	x
x	H	89	0.655850	0.330476	0.310980	x
x	H	90	0.570944	0.270144	0.214584	x
x	C	1	0.135906	0.624521	0.495865	x
x	C	2	0.064658	0.621318	0.578667	x
x	C	3	0.048771	0.553450	0.278143	x
x	C	4	0.972686	0.546380	0.353114	x
x	C	5	0.983002	0.581946	0.506882	x
x	C	6	0.889560	0.504572	0.273106	x
x	C	7	0.041509	0.520967	0.117782	x

x	C	8	0.957400	0.479143	0.043131	x
x	C	9	0.881893	0.471038	0.124126	x
x	C	10	0.951774	0.446296	0.888326	x
x	C	11	0.027027	0.456868	0.815224	x
x	C	12	0.107684	0.501763	0.897283	x
x	C	13	0.820398	0.989904	0.456485	x
x	C	14	0.751456	0.968783	0.564455	x
x	C	15	0.724861	0.897289	0.265785	x
x	C	16	0.650701	0.869709	0.367249	x
x	C	17	0.666635	0.907643	0.519959	x
x	C	18	0.564522	0.805236	0.314151	x
x	C	19	0.711709	0.859593	0.108530	x
x	C	20	0.625409	0.793965	0.061662	x
x	C	21	0.552483	0.767968	0.167320	x
x	C	22	0.615119	0.757141	0.908770	x
x	C	23	0.688037	0.785371	0.812124	x
x	C	24	0.770767	0.851270	0.868415	x
x	C	25	0.839903	0.324408	0.505938	x
x	C	26	0.900078	0.313939	0.410989	x
x	C	27	0.852765	0.244389	0.710561	x
x	C	28	0.912423	0.227989	0.622773	x
x	C	29	0.935463	0.264705	0.469306	x
x	C	30	0.945886	0.175540	0.690042	x
x	C	31	0.828952	0.209762	0.869910	x
x	C	32	0.861749	0.155952	0.930926	x
x	C	33	0.920666	0.139820	0.837896	x
x	C	34	0.833891	0.119843	0.083900	x
x	C	35	0.778661	0.139618	0.169305	x
x	C	36	0.752366	0.196280	0.101403	x
x	C	37	0.375468	0.511378	0.162535	x
x	C	38	0.378682	0.443340	0.245344	x
x	C	39	0.446535	0.495315	0.944809	x
x	C	40	0.453615	0.426307	0.019786	x
x	C	41	0.418053	0.401056	0.173555	x
x	C	42	0.495420	0.384985	0.939781	x
x	C	43	0.479017	0.520534	0.784446	x
x	C	44	0.520856	0.478259	0.709810	x
x	C	45	0.528957	0.410856	0.790805	x
x	C	46	0.553712	0.505481	0.555011	x
x	C	47	0.543126	0.570150	0.481891	x
x	C	48	0.498206	0.605892	0.563927	x
x	C	49	0.010078	0.830471	0.123152	x
x	C	50	0.031216	0.782669	0.231133	x
x	C	51	0.102690	0.827549	0.932448	x
x	C	52	0.130282	0.780982	0.033918	x
x	C	53	0.092356	0.758988	0.186633	x
x	C	54	0.194765	0.759287	0.980829	x
x	C	55	0.140384	0.852091	0.775193	x
x	C	56	0.206031	0.831441	0.728339	x
x	C	57	0.232040	0.784525	0.834005	x
x	C	58	0.242850	0.857972	0.575444	x
x	C	59	0.214599	0.902637	0.478785	x
x	C	60	0.148686	0.919449	0.535069	x
x	C	61	0.675591	0.515492	0.172617	x
x	C	62	0.686067	0.586135	0.077662	x
x	C	63	0.755622	0.608373	0.377232	x
x	C	64	0.772019	0.684431	0.289446	x

x	C	65	0.735308	0.670755	0.135973	x
x	C	66	0.824451	0.770343	0.356725	x
x	C	67	0.790250	0.619189	0.536583	x
x	C	68	0.844029	0.705797	0.597621	x
x	C	69	0.860154	0.780844	0.504595	x
x	C	70	0.880115	0.714051	0.750615	x
x	C	71	0.860378	0.639052	0.836001	x
x	C	72	0.803767	0.556090	0.768065	x
x	C	73	0.488635	0.864089	0.829198	x
x	C	74	0.556669	0.935343	0.912009	x
x	C	75	0.504701	0.951223	0.611469	x
x	C	76	0.573706	0.027311	0.686449	x
x	C	77	0.598951	0.016999	0.840222	x
x	C	78	0.615023	0.110437	0.606444	x
x	C	79	0.479479	0.958486	0.451108	x
x	C	80	0.521755	0.042598	0.376466	x
x	C	81	0.589157	0.118103	0.457463	x
x	C	82	0.494526	0.048226	0.221669	x
x	C	83	0.429847	0.972972	0.148565	x
x	C	84	0.394102	0.892312	0.230606	x
x	C	85	0.169516	0.179603	0.789819	x
x	C	86	0.217333	0.248544	0.897793	x
x	C	87	0.172448	0.275144	0.599117	x
x	C	88	0.219019	0.349301	0.700586	x
x	C	89	0.241019	0.333366	0.853294	x
x	C	90	0.240710	0.435477	0.647501	x
x	C	91	0.147911	0.288299	0.441860	x
x	C	92	0.168558	0.374593	0.395008	x
x	C	93	0.215468	0.447516	0.500681	x
x	C	94	0.142030	0.384883	0.242111	x
x	C	95	0.097363	0.311966	0.145451	x
x	C	96	0.080553	0.229241	0.201731	x
x	C	97	0.484508	0.160087	0.839290	x
x	C	98	0.413865	0.099928	0.744322	x
x	C	99	0.391623	0.147229	0.043902	x
x	C	100	0.315566	0.087581	0.956102	x
x	C	101	0.329244	0.064554	0.802625	x
x	C	102	0.229654	0.054108	0.023375	x
x	C	103	0.380803	0.171030	0.203258	x
x	C	104	0.294196	0.138232	0.264274	x
x	C	105	0.219150	0.079316	0.171237	x
x	C	106	0.285946	0.166083	0.417255	x
x	C	107	0.360950	0.221321	0.502655	x
x	C	108	0.443907	0.247616	0.434753	x
x	N	1	0.128544	0.591698	0.350553	x
x	N	2	0.115263	0.532481	0.044081	x
x	N	3	0.808074	0.955855	0.311663	x
x	N	4	0.782696	0.887325	0.011845	x
x	N	5	0.816705	0.290953	0.650856	x
x	N	6	0.775834	0.229704	0.955997	x
x	N	7	0.408276	0.536833	0.017212	x
x	N	8	0.467485	0.582757	0.710725	x
x	N	9	0.044115	0.852186	0.978320	x
x	N	10	0.112631	0.895325	0.678498	x
x	N	11	0.709054	0.525749	0.317528	x
x	N	12	0.770343	0.546134	0.622657	x
x	N	13	0.463184	0.871447	0.683875	x

```
x  N          14         0.417248   0.884731   0.377398   x
x  N          15         0.147802   0.191931   0.644991   x
x  N          16         0.104681   0.217314   0.345158   x
x  N          17         0.474248   0.183284   0.984207   x
x  N          18         0.453859   0.224137   0.289356   x
x  O           1         0.299633   0.656843   0.216322   x
x  O           2         0.968114   0.002748   0.085457   x
x  O           3         0.698406   0.334947   0.873543   x
x  O           4         0.343280   0.643001   0.883078   x
x  O           5         0.997243   0.965424   0.752147   x
x  O           6         0.665213   0.363522   0.540155   x
x  O           7         0.357147   0.700357   0.549674   x
x  O           8         0.034590   0.031902   0.418843   x
x  O           9         0.636465   0.301711   0.206806   x
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```

Compound **B1** – (PHN)(*p*-DITFB)

Lattice parameters(A)		Cell Angles	
a =	4.561800	alpha =	90.000000
b =	16.246201	beta =	91.259003
c =	24.087999	gamma =	90.000000

Cell Contents

Element	Atom Number	Fractional coordinates of atoms u	v	w
H	1	0.750847	0.290118	0.350973
H	2	0.614195	0.414687	0.295564
H	3	0.820682	0.431124	0.199932
H	4	0.138253	0.376919	0.126567
H	5	0.475935	0.269570	0.092633
H	6	0.752428	0.140455	0.109514
H	7	0.885919	0.023445	0.173748
H	8	0.665426	0.020620	0.268332
H	9	0.249147	0.790119	0.149026
H	10	0.385805	0.914687	0.204435
H	11	0.179320	0.931124	0.300068
H	12	0.861750	0.876920	0.373432
H	13	0.524066	0.769571	0.407367
H	14	0.247572	0.640457	0.390486
H	15	0.114083	0.523445	0.326253
H	16	0.334580	0.520619	0.231669
H	17	0.249145	0.709882	0.649026
H	18	0.385800	0.585312	0.704434
H	19	0.179317	0.568875	0.800067
H	20	0.861751	0.623079	0.873433
H	21	0.524069	0.730428	0.907367
H	22	0.247574	0.859543	0.890486
H	23	0.114086	0.976555	0.826253
H	24	0.334585	0.979381	0.731669
H	25	0.750853	0.209882	0.850974
H	26	0.614196	0.085313	0.795565
H	27	0.820681	0.068876	0.699933
H	28	0.138248	0.123081	0.626568
H	29	0.475930	0.230430	0.592633
H	30	0.752425	0.359544	0.609515
H	31	0.885917	0.476555	0.673748
H	32	0.665420	0.479380	0.768332
C	1	0.145463	0.250812	0.241881
C	2	0.843762	0.299965	0.310088
C	3	0.764270	0.369626	0.278533
C	4	0.878988	0.378720	0.226357
C	5	0.073376	0.318506	0.206450
C	6	0.196419	0.324116	0.152492
C	7	0.383134	0.265154	0.133907
C	8	0.463650	0.196810	0.168367

x	C	9	0.659707	0.135517	0.150681	x
x	C	10	0.733274	0.071451	0.185965	x
x	C	11	0.608414	0.069764	0.238946	x
x	C	12	0.348100	0.188894	0.222565	x
x	C	13	0.957023	0.550807	0.047454	x
x	C	14	0.821458	0.474329	0.041889	x
x	C	15	0.135235	0.575689	0.004284	x
x	C	16	0.417744	0.422510	0.477426	x
x	C	17	0.314187	0.449085	0.528321	x
x	C	18	0.605232	0.474929	0.449338	x
x	C	19	0.854536	0.750813	0.258118	x
x	C	20	0.156232	0.799966	0.189911	x
x	C	21	0.235730	0.869627	0.221466	x
x	C	22	0.121013	0.878720	0.273642	x
x	C	23	0.926624	0.818507	0.293550	x
x	C	24	0.803583	0.824117	0.347507	x
x	C	25	0.616866	0.765155	0.366092	x
x	C	26	0.536347	0.696811	0.331632	x
x	C	27	0.340292	0.635518	0.349319	x
x	C	28	0.266728	0.571451	0.314035	x
x	C	29	0.391588	0.569764	0.261054	x
x	C	30	0.651898	0.688895	0.277434	x
x	C	31	0.042982	0.050808	0.452546	x
x	C	32	0.178543	0.974329	0.458111	x
x	C	33	0.864771	0.075690	0.495717	x
x	C	34	0.582254	0.922509	0.022574	x
x	C	35	0.685811	0.949084	0.971679	x
x	C	36	0.394766	0.974928	0.050662	x
x	C	37	0.854536	0.749187	0.758118	x
x	C	38	0.156231	0.700034	0.689911	x
x	C	39	0.235726	0.630372	0.721465	x
x	C	40	0.121009	0.621279	0.773642	x
x	C	41	0.926623	0.681493	0.793550	x
x	C	42	0.803583	0.675883	0.847507	x
x	C	43	0.616868	0.734845	0.866093	x
x	C	44	0.536350	0.803189	0.831633	x
x	C	45	0.340295	0.864482	0.849320	x
x	C	46	0.266732	0.928549	0.814036	x
x	C	47	0.391592	0.930236	0.761055	x
x	C	48	0.651900	0.811105	0.777435	x
x	C	49	0.042981	0.449192	0.952546	x
x	C	50	0.178543	0.525671	0.958110	x
x	C	51	0.864772	0.424310	0.995717	x
x	C	52	0.582253	0.577492	0.522574	x
x	C	53	0.685811	0.550916	0.471679	x
x	C	54	0.394765	0.525072	0.550662	x
x	C	55	0.145464	0.249188	0.741882	x
x	C	56	0.843766	0.200035	0.810089	x
x	C	57	0.764271	0.130373	0.778534	x
x	C	58	0.878988	0.121280	0.726358	x
x	C	59	0.073376	0.181494	0.706451	x
x	C	60	0.196416	0.175884	0.652493	x
x	C	61	0.383132	0.234846	0.633908	x
x	C	62	0.463649	0.303190	0.668368	x
x	C	63	0.659705	0.364483	0.650681	x
x	C	64	0.733271	0.428549	0.685965	x
x	C	65	0.608411	0.430236	0.738946	x

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x  C          66         0.348100   0.311106   0.722566   x
x  C          67         0.957019   0.949193   0.547455   x
x  C          68         0.821456   0.025672   0.541889   x
x  C          69         0.135229   0.924311   0.504284   x
x  C          70         0.417746   0.077491   0.977426   x
x  C          71         0.314189   0.050916   0.028321   x
x  C          72         0.605233   0.025072   0.949338   x
x  N           1         0.029184   0.242776   0.292940   x
x  N           2         0.420986   0.125802   0.256825   x
x  N           3         0.970813   0.742777   0.207060   x
x  N           4         0.579015   0.625802   0.243175   x
x  N           5         0.970813   0.757223   0.707060   x
x  N           6         0.579017   0.874198   0.743175   x
x  N           7         0.029186   0.257224   0.792941   x
x  N           8         0.420985   0.374198   0.756825   x
x  F           1         0.642457   0.446430   0.081967   x
x  F           2         0.273008   0.649297   0.006365   x
x  F           3         0.130715   0.400982   0.557303   x
x  F           4         0.712939   0.453409   0.399633   x
x  F           5         0.357542   0.946430   0.418033   x
x  F           6         0.727002   0.149300   0.493636   x
x  F           7         0.869279   0.900981   0.942696   x
x  F           8         0.287061   0.953409   0.100367   x
x  F           9         0.357542   0.553571   0.918032   x
x  F          10         0.727004   0.350701   0.993636   x
x  F          11         0.869280   0.599019   0.442696   x
x  F          12         0.287059   0.546592   0.600367   x
x  F          13         0.642455   0.053570   0.581967   x
x  F          14         0.272999   0.850702   0.506364   x
x  F          15         0.130719   0.099019   0.057304   x
x  F          16         0.712940   0.046591   0.899632   x
x  I           1         0.910977   0.622869   0.120837   x
x  I           2         0.291696   0.307226   0.444705   x
x  I           3         0.089025   0.122870   0.379163   x
x  I           4         0.708304   0.807225   0.055295   x
x  I           5         0.089023   0.377131   0.879162   x
x  I           6         0.708302   0.692776   0.555295   x
x  I           7         0.910972   0.877131   0.620838   x
x  I           8         0.291698   0.192775   0.944705   x
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Compound **B2 –** (PHN)(*sym*-TFTIB)

Lattice parameters(A)		Cell Angles	
a =	8.644500	alpha =	90.000000
b =	14.047200	beta =	97.662003
c =	15.814700	gamma =	90.000000

Cell Contents

Element	Atom Number	Fractional coordinates of atoms u	v	w
H	1	0.180862	0.384733	0.748476
H	2	0.096920	0.312017	0.878884
H	3	0.148451	0.401723	1.017539
H	4	0.259224	0.543673	1.096458
H	5	0.403622	0.696136	1.098374
H	6	0.547680	0.814483	1.023830
H	7	0.634830	0.872521	0.887133
H	8	0.586183	0.768647	0.757859
H	9	0.819139	-0.115268	0.751524
H	10	0.903082	-0.187982	0.621115
H	11	0.851550	-0.098276	0.482462
H	12	0.740778	0.043673	0.403543
H	13	0.596378	0.196136	0.401627
H	14	0.452322	0.314482	0.476171
H	15	0.365170	0.372522	0.612866
H	16	0.413815	0.268648	0.742140
H	17	0.819140	0.615268	0.251524
H	18	0.903083	0.687983	0.121115
H	19	0.851551	0.598276	-0.017540
H	20	0.740778	0.456327	-0.096457
H	21	0.596378	0.303863	-0.098373
H	22	0.452324	0.185517	-0.023830
H	23	0.365170	0.127478	0.112866
H	24	0.413812	0.231353	0.242140
H	25	0.180862	1.115268	0.248475
H	26	0.096920	1.187983	0.378884
H	27	0.148451	1.098277	0.517539
H	28	0.259224	0.956328	0.596456
H	29	0.403622	0.803865	0.598373
H	30	0.547680	0.685518	0.523830
H	31	0.634829	0.627479	0.387134
H	32	0.586180	0.731351	0.257858
C	1	0.763720	0.444111	0.645135
C	2	0.842829	0.363852	0.679787
C	3	0.923448	0.303383	0.630923
C	4	0.919232	0.323609	0.544281
C	5	0.836682	0.400810	0.505653
C	6	0.762578	0.460351	0.558219
C	7	0.208043	0.420127	0.810245
C	8	0.159059	0.379541	0.883505
C	9	0.188131	0.428784	0.959431
C	10	0.270697	0.515598	0.962142

x	C	11	0.301935	0.569991	1.038906	x
x	C	12	0.382173	0.653640	1.040145	x
x	C	13	0.439671	0.687680	0.965044	x
x	C	14	0.523486	0.773854	0.964756	x
x	C	15	0.572889	0.805275	0.890149	x
x	C	16	0.544210	0.747259	0.817257	x
x	C	17	0.412880	0.635050	0.887346	x
x	C	18	0.321951	0.548357	0.885150	x
x	C	19	0.236281	0.944111	0.854866	x
x	C	20	0.157172	0.863852	0.820213	x
x	C	21	0.076555	0.803382	0.869078	x
x	C	22	0.080771	0.823608	0.955719	x
x	C	23	0.163319	0.900810	0.994349	x
x	C	24	0.237421	0.960351	0.941782	x
x	C	25	0.791957	-0.079873	0.689755	x
x	C	26	0.840941	-0.120459	0.616496	x
x	C	27	0.811869	-0.071216	0.540570	x
x	C	28	0.729305	0.015597	0.537858	x
x	C	29	0.698066	0.069991	0.461095	x
x	C	30	0.617828	0.153640	0.459856	x
x	C	31	0.560329	0.187680	0.534957	x
x	C	32	0.476514	0.273855	0.535245	x
x	C	33	0.427112	0.305277	0.609851	x
x	C	34	0.455788	0.247260	0.682742	x
x	C	35	0.587119	0.135050	0.612653	x
x	C	36	0.678048	0.048356	0.614850	x
x	C	37	0.236279	0.555888	0.354866	x
x	C	38	0.157171	0.636146	0.320214	x
x	C	39	0.076553	0.696617	0.369078	x
x	C	40	0.080770	0.676391	0.455719	x
x	C	41	0.163318	0.599190	0.494349	x
x	C	42	0.237421	0.539649	0.441782	x
x	C	43	0.791956	0.579874	0.189755	x
x	C	44	0.840942	0.620459	0.116495	x
x	C	45	0.811870	0.571216	0.040569	x
x	C	46	0.729304	0.484403	0.037858	x
x	C	47	0.698066	0.430009	-0.038906	x
x	C	48	0.617829	0.346360	-0.040145	x
x	C	49	0.560329	0.312321	0.034956	x
x	C	50	0.476514	0.226146	0.035244	x
x	C	51	0.427113	0.194723	0.109851	x
x	C	52	0.455786	0.252741	0.182742	x
x	C	53	0.587120	0.364950	0.112653	x
x	C	54	0.678049	0.451644	0.114851	x
x	C	55	0.763718	0.055890	0.145134	x
x	C	56	0.842827	0.136148	0.179785	x
x	C	57	0.923448	0.196617	0.130922	x
x	C	58	0.919230	0.176391	0.044281	x
x	C	59	0.836682	0.099190	0.005652	x
x	C	60	0.762578	0.039650	0.058219	x
x	C	61	0.208043	1.079874	0.310245	x
x	C	62	0.159060	1.120459	0.383505	x
x	C	63	0.188131	1.071216	0.459431	x
x	C	64	0.270696	0.984402	0.462143	x
x	C	65	0.301935	0.930009	0.538906	x
x	C	66	0.382172	0.846360	0.540145	x
x	C	67	0.439669	0.812320	0.465043	x

```
x  C          68         0.523485   0.726146   0.464756   x
x  C          69         0.572887   0.694725   0.390149   x
x  C          70         0.544210   0.752740   0.317257   x
x  C          71         0.412879   0.864950   0.387346   x
x  C          72         0.321951   0.951643   0.385151   x
x  N           1         0.285493   0.501801   0.809951   x
x  N           2         0.470122   0.664165   0.815639   x
x  N           3         0.714506   0.001800   0.690048   x
x  N           4         0.529881   0.164167   0.684361   x
x  N           5         0.714507   0.498200   0.190049   x
x  N           6         0.529881   0.335833   0.184362   x
x  N           7         0.285492   0.998199   0.309952   x
x  N           8         0.470118   0.835834   0.315638   x
x  F           1         0.841370   0.344189   0.763342   x
x  F           2         0.996420   0.265751   0.496044   x
x  F           3         0.683567   0.536686   0.522924   x
x  F           4         0.158631   0.844189   0.736658   x
x  F           5         0.003583   0.765749   1.003955   x
x  F           6         0.316431   1.036687   0.977076   x
x  F           7         0.158629   0.655809   0.236658   x
x  F           8         0.003583   0.734250   0.503956   x
x  F           9         0.316432   0.463314   0.477076   x
x  F          10         0.841367   0.155811   0.263339   x
x  F          11         0.996420   0.234248  -0.003955   x
x  F          12         0.683566  -0.036684   0.022924   x
x  I           1         0.636144   0.534198   0.718198   x
x  I           2         1.054802   0.187465   0.687237   x
x  I           3         0.806210   0.423482   0.372356   x
x  I           4         0.363856   1.034200   0.781802   x
x  I           5        -0.054803   0.687466   0.812762   x
x  I           6         0.193787   0.923481   1.127644   x
x  I           7         0.363855   0.465800   0.281802   x
x  I           8        -0.054803   0.812533   0.312763   x
x  I           9         0.193789   0.576519   0.627644   x
x  I          10         0.636144  -0.034199   0.218198   x
x  I          11         1.054800   0.312535   0.187236   x
x  I          12         0.806211   0.076518  -0.127646   x
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Compound **C** – (TMP)

Lattice parameters(A)		Cell Angles	
a =	8.331000	alpha =	90.000000
b =	9.225000	beta =	90.000000
c =	10.148000	gamma =	90.000000

Cell Contents

Element	Atom Number	Fractional coordinates of atoms u	v	w
H	1	0.102211	0.355610	0.009410
H	2	0.050359	0.311789	0.175451
H	3	0.896618	0.350990	0.061347
H	4	0.893734	0.129736	0.302426
H	5	0.744402	0.999291	0.259792
H	6	0.735575	0.180651	0.196277
H	7	0.397789	0.644390	0.509410
H	8	0.449641	0.688211	0.675451
H	9	0.603382	0.649010	0.561347
H	10	0.606266	0.870264	0.802426
H	11	0.755598	0.000709	0.759792
H	12	0.764425	0.819349	0.696277
H	13	0.897789	0.855610	0.490590
H	14	0.949641	0.811789	0.324549
H	15	0.103382	0.850990	0.438653
H	16	0.106266	0.629736	0.197574
H	17	0.255598	0.499291	0.240208
H	18	0.264425	0.680651	0.303723
H	19	0.602211	0.144390	0.990590
H	20	0.550359	0.188211	0.824549
H	21	0.396618	0.149010	0.938653
H	22	0.393734	0.370264	0.697574
H	23	0.244402	0.500708	0.740208
H	24	0.235575	0.319349	0.803723
H	25	0.897789	0.644390	0.990590
H	26	0.949641	0.688211	0.824549
H	27	0.103382	0.649010	0.938653
H	28	0.106266	0.870264	0.697574
H	29	0.255598	0.000709	0.740208
H	30	0.264425	0.819349	0.803723
H	31	0.602211	0.355610	0.490590
H	32	0.550359	0.311789	0.324549
H	33	0.396618	0.350990	0.438653
H	34	0.393734	0.129736	0.197574
H	35	0.244402	0.999291	0.240208
H	36	0.235575	0.180651	0.303723
H	37	0.102211	0.144390	0.509410
H	38	0.050359	0.188211	0.675451
H	39	0.896618	0.149010	0.561347
H	40	0.893734	0.370264	0.802426
H	41	0.744402	0.500708	0.759792
H	42	0.735575	0.319349	0.696277

```
x  H          43        0.397789   0.855610   0.009410   x
x  H          44        0.449641   0.811789   0.175451   x
x  H          45        0.603382   0.850990   0.061347   x
x  H          46        0.606266   0.629736   0.302426   x
x  H          47        0.755598   0.499291   0.259792   x
x  H          48        0.764425   0.680651   0.196277   x
x  C           1        0.006828   0.142127   0.033724   x
x  C           2        0.912634   0.042870   0.105703   x
x  C           3        0.014976   0.298771   0.071564   x
x  C           4        0.815844   0.090186   0.222378   x
x  C           5        0.493172   0.857873   0.533724   x
x  C           6        0.587366   0.957130   0.605703   x
x  C           7        0.485024   0.701229   0.571564   x
x  C           8        0.684156   0.909813   0.722378   x
x  C           9        0.993172   0.642127   0.466276   x
x  C          10        0.087366   0.542870   0.394297   x
x  C          11        0.985024   0.798770   0.428436   x
x  C          12        0.184156   0.590186   0.277622   x
x  C          13        0.506829   0.357873   0.966276   x
x  C          14        0.412634   0.457130   0.894297   x
x  C          15        0.514976   0.201229   0.928436   x
x  C          16        0.315844   0.409813   0.777622   x
x  C          17        0.993171   0.857873   0.966276   x
x  C          18        0.087366   0.957130   0.894297   x
x  C          19        0.985024   0.701229   0.928436   x
x  C          20        0.184156   0.909814   0.777622   x
x  C          21        0.506828   0.142127   0.466276   x
x  C          22        0.412634   0.042870   0.394297   x
x  C          23        0.514976   0.298771   0.428436   x
x  C          24        0.315844   0.090187   0.277622   x
x  C          25        0.006828   0.357873   0.533724   x
x  C          26        0.912634   0.457130   0.605703   x
x  C          27        0.014976   0.201230   0.571564   x
x  C          28        0.815844   0.409813   0.722378   x
x  C          29        0.493171   0.642127   0.033724   x
x  C          30        0.587366   0.542870   0.105703   x
x  C          31        0.485024   0.798771   0.071564   x
x  C          32        0.684156   0.590187   0.222378   x
x  N           1        0.092688   0.097784   0.928962   x
x  N           2        0.407312   0.902217   0.428962   x
x  N           3        0.907312   0.597784   0.571038   x
x  N           4        0.592689   0.402217   0.071038   x
x  N           5        0.907312   0.902216   0.071038   x
x  N           6        0.592688   0.097783   0.571038   x
x  N           7        0.092688   0.402216   0.428962   x
x  N           8        0.407312   0.597783   0.928962   x
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Compound **C1** – (TMP)(*p*-DITFB)

Lattice parameters(A)		Cell Angles	
a =	11.057300	alpha =	90.000000
b =	5.703100	beta =	106.907997
c =	14.013600	gamma =	90.000000

Cell Contents

Element	Atom Number	Fractional coordinates of atoms u	v	w
H	1	0.269299	0.769566	0.157801
H	2	0.186258	0.893780	0.237217
H	3	0.276404	0.076060	0.183123
H	4	0.036509	0.557680	0.849925
H	5	0.871223	0.620970	0.811684
H	6	0.974744	0.793729	0.766405
H	7	0.730693	0.269604	0.342188
H	8	0.813738	0.393856	0.262783
H	9	0.723600	0.576124	0.316886
H	10	0.963460	0.057702	0.650069
H	11	0.128758	0.120898	0.688298
H	12	0.025274	0.293688	0.733596
H	13	0.730701	0.230433	0.842199
H	14	0.813743	0.106220	0.762783
H	15	0.723596	0.923939	0.816877
H	16	0.963492	0.442320	0.150076
H	17	0.128777	0.379031	0.188316
H	18	0.025257	0.206271	0.233595
H	19	0.269306	0.730396	0.657811
H	20	0.186262	0.606144	0.737217
H	21	0.276399	0.423876	0.683114
H	22	0.036540	0.942299	0.349931
H	23	0.871241	0.879103	0.311702
H	24	0.974725	0.706312	0.266403
C	1	0.409669	0.179038	0.997581
C	2	0.408108	0.051366	0.912502
C	3	0.503311	0.124195	0.085338
C	4	0.101910	0.960418	0.080295
C	5	0.985089	0.858008	0.920092
C	6	0.214296	0.921295	0.168921
C	7	0.966207	0.698481	0.832363
C	8	0.590323	0.679044	0.502412
C	9	0.591884	0.551399	0.587498
C	10	0.496690	0.624170	0.414656
C	11	0.898086	0.460439	0.419705
C	12	0.014911	0.357996	0.579907
C	13	0.785697	0.421343	0.331079
C	14	0.033786	0.198455	0.667630
C	15	0.590331	0.820963	0.002418
C	16	0.591892	0.948635	0.087498
C	17	0.496689	0.875805	0.914662
C	18	0.898091	0.039582	0.919705

```
x  C          19         0.014912   0.141992   0.079908   x
x  C          20         0.785704   0.078705   0.831079   x
x  C          21         0.033794   0.301519   0.167637   x
x  C          22         0.409676   0.320955   0.497588   x
x  C          23         0.408116   0.448601   0.412502   x
x  C          24         0.503310   0.375827   0.585344   x
x  C          25         0.101913   0.539561   0.580295   x
x  C          26         0.985088   0.642005   0.420093   x
x  C          27         0.214302   0.578657   0.668921   x
x  C          28         0.966213   0.801547   0.332370   x
x  N           1         0.085469   0.821286   1.000048   x
x  N           2         0.914530   0.321298   0.499950   x
x  N           3         0.914532   0.178715  -0.000047   x
x  N           4         0.085470   0.678703   0.500050   x
x  F           1         0.318911   0.094619   0.825309   x
x  F           2         0.510963   0.242933   0.170273   x
x  F           3         0.681071   0.594702   0.674692   x
x  F           4         0.489038   0.742884   0.329715   x
x  F           5         0.681090   0.905383   0.174691   x
x  F           6         0.489036   0.757066   0.829727   x
x  F           7         0.318930   0.405297   0.325309   x
x  F           8         0.510963   0.257112   0.670286   x
x  I           1         0.275734   0.448047   0.995147   x
x  I           2         0.724256   0.948058   0.504845   x
x  I           3         0.724266   0.551953   0.004853   x
x  I           4         0.275744   0.051942   0.495155   x
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Compound **C2** – (TMP)(*sym*-TFTIB)

Lattice parameters(A)		Cell Angles	
a =	7.981800	alpha =	90.000000
b =	26.704599	beta =	115.398003
c =	9.222000	gamma =	90.000000

Cell Contents

Element	Atom Number	Fractional coordinates of atoms u	v	w
H	1	0.061976	0.532908	0.825962
H	2	0.062071	0.546198	0.014772
H	3	0.253938	0.564047	0.979297
H	4	0.351428	0.660910	0.112200
H	5	0.227372	0.618773	0.178263
H	6	0.195509	0.684669	0.186351
H	7	0.681875	0.667727	0.397537
H	8	0.513662	0.677993	0.471164
H	9	0.579160	0.615529	0.446618
H	10	0.797793	0.776241	0.767549
H	11	0.591961	0.744599	0.634600
H	12	0.766681	0.759056	0.571812
H	13	0.938024	0.032908	0.674039
H	14	0.937929	0.046198	0.485229
H	15	0.746061	0.064047	0.520704
H	16	0.648573	0.160910	0.387800
H	17	0.772629	0.118773	0.321738
H	18	0.804491	0.184668	0.313650
H	19	0.318125	0.167727	0.102462
H	20	0.486338	0.177993	0.028836
H	21	0.420840	0.115530	0.053381
H	22	0.202208	0.276241	0.732451
H	23	0.408038	0.244599	0.865400
H	24	0.233319	0.259056	0.928187
H	25	0.938023	0.467092	0.174038
H	26	0.937929	0.453802	0.985229
H	27	0.746062	0.435953	0.020703
H	28	0.648573	0.339090	0.887800
H	29	0.772629	0.381227	0.821738
H	30	0.804491	0.315332	0.813649
H	31	0.318126	0.332273	0.602462
H	32	0.486338	0.322007	0.528836
H	33	0.420841	0.384470	0.553382
H	34	0.202207	0.223758	0.232451
H	35	0.408038	0.255401	0.365400
H	36	0.233319	0.240944	0.428188
H	37	0.061977	0.967092	0.325961
H	38	0.062071	0.953802	0.514771
H	39	0.253938	0.935953	0.479296
H	40	0.351428	0.839090	0.612200
H	41	0.227372	0.881227	0.678263
H	42	0.195509	0.815332	0.686351

x	H	43	0.681875	0.832273	0.897538	x
x	H	44	0.513662	0.822007	0.971164	x
x	H	45	0.579159	0.884470	0.946618	x
x	H	46	0.797793	0.723759	0.267549	x
x	H	47	0.591961	0.755401	0.134599	x
x	H	48	0.766681	0.740944	0.071812	x
x	C	1	0.674362	0.451090	0.381381	x
x	C	2	0.530691	0.450598	0.226831	x
x	C	3	0.476401	0.407051	0.134328	x
x	C	4	0.568022	0.362581	0.202793	x
x	C	5	0.710781	0.360451	0.357438	x
x	C	6	0.761028	0.405449	0.442123	x
x	C	7	0.102403	0.560651	0.922540	x
x	C	8	0.009065	0.609593	0.858114	x
x	C	9	0.063083	0.653943	0.949849	x
x	C	10	0.216946	0.654384	0.115701	x
x	C	11	0.629837	0.653749	0.482894	x
x	C	12	0.781614	0.653808	0.649757	x
x	C	13	0.836411	0.698226	0.740986	x
x	C	14	0.742988	0.747048	0.675602	x
x	C	15	0.325639	0.951089	0.118619	x
x	C	16	0.469308	0.950598	0.273169	x
x	C	17	0.523599	0.907051	0.365672	x
x	C	18	0.431979	0.862581	0.297208	x
x	C	19	0.289219	0.860451	0.142562	x
x	C	20	0.238972	0.905449	0.057876	x
x	C	21	0.897597	0.060651	0.577461	x
x	C	22	0.990934	0.109593	0.641887	x
x	C	23	0.936916	0.153943	0.550151	x
x	C	24	0.783054	0.154384	0.384299	x
x	C	25	0.370164	0.153749	0.017107	x
x	C	26	0.218387	0.153808	0.850244	x
x	C	27	0.163591	0.198226	0.759014	x
x	C	28	0.257013	0.247048	0.824398	x
x	C	29	0.325638	0.548911	0.618619	x
x	C	30	0.469308	0.549402	0.773169	x
x	C	31	0.523599	0.592949	0.865672	x
x	C	32	0.431979	0.637419	0.797207	x
x	C	33	0.289219	0.639549	0.642562	x
x	C	34	0.238971	0.594551	0.557876	x
x	C	35	0.897597	0.439349	0.077460	x
x	C	36	0.990934	0.390407	0.141886	x
x	C	37	0.936917	0.346057	0.050151	x
x	C	38	0.783054	0.345616	0.884300	x
x	C	39	0.370164	0.346251	0.517107	x
x	C	40	0.218387	0.346192	0.350244	x
x	C	41	0.163591	0.301774	0.259014	x
x	C	42	0.257013	0.252952	0.324398	x
x	C	43	0.674362	0.048910	0.881381	x
x	C	44	0.530692	0.049402	0.726831	x
x	C	45	0.476401	0.092949	0.634328	x
x	C	46	0.568021	0.137419	0.702793	x
x	C	47	0.710781	0.139549	0.857438	x
x	C	48	0.761028	0.094551	0.942123	x
x	C	49	0.102402	0.939349	0.422539	x
x	C	50	0.009065	0.890407	0.358114	x
x	C	51	0.063082	0.846057	0.449849	x

```
x  C          52         0.216946   0.845616   0.615700   x
x  C          53         0.629836   0.846251   0.982893   x
x  C          54         0.781613   0.846192   0.149757   x
x  C          55         0.836410   0.801774   0.240986   x
x  C          56         0.742987   0.752952   0.175602   x
x  N           1         0.869322   0.610374   0.709581   x
x  N           2         0.976855   0.697464   0.889027   x
x  N           3         0.130678   0.110374   0.790419   x
x  N           4         0.023145   0.197464   0.610973   x
x  N           5         0.130678   0.389626   0.290419   x
x  N           6         0.023145   0.302536   0.110973   x
x  N           7         0.869321   0.889626   0.209581   x
x  N           8         0.976855   0.802536   0.389027   x
x  F           1         0.899547   0.404652   0.592739   x
x  F           2         0.441457   0.493699   0.163775   x
x  F           3         0.515943   0.319945   0.115775   x
x  F           4         0.100451   0.904652   0.907261   x
x  F           5         0.558543   0.993698   0.336225   x
x  F           6         0.484058   0.819945   0.384225   x
x  F           7         0.100452   0.595348   0.407262   x
x  F           8         0.558543   0.506301   0.836225   x
x  F           9         0.484057   0.680055   0.884225   x
x  F          10         0.899548   0.095348   0.092739   x
x  F          11         0.441457   0.006301   0.663775   x
x  F          12         0.515943   0.180055   0.615775   x
x  I           1         0.756540   0.518211   0.519293   x
x  I           2         0.268452   0.408809   0.897650   x
x  I           3         0.842172   0.291095   0.460327   x
x  I           4         0.243461   0.018211   0.980706   x
x  I           5         0.731548   0.908809   0.602349   x
x  I           6         0.157827   0.791095   0.039672   x
x  I           7         0.243461   0.481789   0.480707   x
x  I           8         0.731548   0.591191   0.102349   x
x  I           9         0.157828   0.708905   0.539672   x
x  I          10         0.756540   0.981789   0.019293   x
x  I          11         0.268452   0.091191   0.397650   x
x  I          12         0.842173   0.208905   0.960327   x
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Compound **D** - (UTP)

Lattice parameters(A)		Cell Angles	
a =	7.021000	alpha =	90.000000
b =	7.021000	beta =	90.000000
c =	7.021000	gamma =	90.000000

Element	Atom Number	Fractional coordinates of atoms u	v	w
H	1	0.329997	0.091016	0.908984
H	2	0.829997	0.591016	0.408984
H	3	0.670003	0.908984	0.908984
H	4	0.170003	0.408984	0.408984
H	5	0.670003	0.091016	0.091016
H	6	0.170003	0.591016	0.591016
H	7	0.329997	0.908984	0.091016
H	8	0.829997	0.408984	0.591016
H	9	0.908984	0.329997	0.091016
H	10	0.408984	0.829997	0.591016
H	11	0.908984	0.670003	0.908984
H	12	0.408984	0.170003	0.408984
H	13	0.091016	0.670003	0.091016
H	14	0.591016	0.170003	0.591016
H	15	0.091016	0.329997	0.908984
H	16	0.591016	0.829997	0.408984
H	17	0.091016	0.908984	0.329997
H	18	0.591016	0.408984	0.829997
H	19	0.908984	0.908984	0.670003
H	20	0.408984	0.408984	0.170003
H	21	0.091016	0.091016	0.670003
H	22	0.591016	0.591016	0.170003
H	23	0.908984	0.091016	0.329997
H	24	0.408984	0.591016	0.829997
C	1	0.240381	0.000000	0.000000
C	2	0.740381	0.500000	0.500000
C	3	0.759619	0.000000	0.000000
C	4	0.259619	0.500000	0.500000
C	5	0.000000	0.240381	0.000000
C	6	0.500000	0.740381	0.500000
C	7	0.000000	0.759619	0.000000
C	8	0.500000	0.259619	0.500000
C	9	0.000000	0.000000	0.240381
C	10	0.500000	0.500000	0.740381
C	11	0.000000	0.000000	0.759619
C	12	0.500000	0.500000	0.259619
N	1	0.123601	0.123601	0.123601
N	2	0.623601	0.623601	0.623601
N	3	0.876399	0.876399	0.123601
N	4	0.376399	0.376399	0.623601
N	5	0.876399	0.123601	0.876399
N	6	0.376399	0.623601	0.376399
N	7	0.123601	0.876399	0.876399
N	8	0.623601	0.376399	0.376399

Compound **D1** – (UTP)(*p*-DITFB)

Lattice parameters(A)		Cell Angles	
a =	5.977000	alpha =	90.000000
b =	21.539000	beta =	94.559998
c =	6.313000	gamma =	90.000000

Cell Contents

Element	Atom Number	Fractional coordinates of atoms u	v	w
H	1	0.665513	0.306153	0.052613
H	2	0.671301	0.347370	0.807850
H	3	0.100199	0.305906	0.614270
H	4	0.347914	0.347235	0.554929
H	5	0.677397	0.291610	0.479746
H	6	0.334486	0.806153	0.947388
H	7	0.328699	0.847370	0.192150
H	8	0.899801	0.805906	0.385729
H	9	0.652087	0.847235	0.445071
H	10	0.322605	0.791610	0.520255
H	11	0.334486	0.693847	0.947388
H	12	0.328699	0.652630	0.192150
H	13	0.899801	0.694094	0.385729
H	14	0.652088	0.652765	0.445072
H	15	0.322605	0.708390	0.520256
H	16	0.665513	0.193847	0.052613
H	17	0.671301	0.152630	0.807850
H	18	0.100199	0.194094	0.614270
H	19	0.347914	0.152765	0.554929
H	20	0.677397	0.208390	0.479745
H	21	0.325964	0.250000	0.130723
H	22	0.090504	0.250000	0.935281
H	23	0.674035	0.750000	0.869278
H	24	0.909495	0.750000	0.064718
C	1	0.074978	0.462088	0.335259
C	2	0.187379	0.516398	0.398263
C	3	0.886494	0.446670	0.440064
C	4	0.608274	0.305521	0.882757
C	5	0.284608	0.305616	0.631112
C	6	0.925022	0.962088	0.664740
C	7	0.812620	0.016398	0.601737
C	8	0.113505	0.946670	0.559935
C	9	0.391726	0.805521	0.117244
C	10	0.715393	0.805616	0.368888
C	11	0.925022	0.537912	0.664740
C	12	0.812620	0.483602	0.601737
C	13	0.113506	0.553330	0.559935
C	14	0.391726	0.694479	0.117244
C	15	0.715393	0.694384	0.368888
C	16	0.074978	0.037912	0.335260
C	17	0.187379	0.983602	0.398263
C	18	0.886494	0.053330	0.440064

```
x  C          19         0.608274   0.194479   0.882757   x
x  C          20         0.284608   0.194384   0.631112   x
x  C          21         0.274735   0.250000   0.959423   x
x  C          22         0.613910   0.250000   0.555696   x
x  C          23         0.725264   0.750000   0.040578   x
x  C          24         0.386091   0.750000   0.444304   x
x  N           1         0.359668   0.306746   0.860685   x
x  N           2         0.640332   0.806746   0.139315   x
x  N           3         0.640332   0.693254   0.139315   x
x  N           4         0.359668   0.193254   0.860685   x
x  N           5         0.697123   0.250000   0.782515   x
x  N           6         0.367066   0.250000   0.526625   x
x  N           7         0.302877   0.750000   0.217486   x
x  N           8         0.632935   0.750000   0.473374   x
x  F           1         0.371851   0.534530   0.303156   x
x  F           2         0.769742   0.394061   0.386942   x
x  F           3         0.628148   0.034530   0.696843   x
x  F           4         0.230258   0.894061   0.613057   x
x  F           5         0.628148   0.465470   0.696843   x
x  F           6         0.230258   0.605939   0.613057   x
x  F           7         0.371852   0.965470   0.303156   x
x  F           8         0.769742   0.105939   0.386942   x
x  I           1         0.196570   0.400857   0.103282   x
x  I           2         0.803429   0.900857   0.896718   x
x  I           3         0.803430   0.599143   0.896718   x
x  I           4         0.196570   0.099143   0.103282   x
xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
```

Compound **D2** – (UTP)(*sym*-TFTIB)

Lattice parameters(A)		Cell Angles	
a =	5.884900	alpha =	90.000000
b =	24.903000	beta =	98.863998
c =	6.224700	gamma =	90.000000

Cell Contents

Element	Atom Number	Fractional coordinates of atoms u	v	w
H	1	0.968077	0.951430	0.859286
H	2	0.017994	0.915659	0.110992
H	3	0.466837	0.952061	0.269353
H	4	0.728452	0.915609	0.347822
H	5	0.083380	0.963950	0.448791
H	6	0.604164	0.536027	0.270546
H	7	0.177948	0.451522	0.129560
H	8	0.932603	0.415800	0.191540
H	9	0.583537	0.584197	0.937664
H	10	0.564708	0.549220	0.685634
H	11	0.968077	0.048570	0.859286
H	12	0.017994	0.084342	0.110991
H	13	0.466837	0.047939	0.269353
H	14	0.728452	0.084392	0.347822
H	15	0.083380	0.036050	0.448791
H	16	0.604164	0.463973	0.270546
H	17	0.177948	0.548478	0.129560
H	18	0.932603	0.584200	0.191540
H	19	0.583538	0.415803	0.937664
H	20	0.564708	0.450780	0.685633
H	21	0.616164	0.000000	0.756224
H	22	0.401635	0.000000	0.936019
H	23	0.160442	0.500000	0.802300
H	24	0.906977	0.500000	0.602127
C	1	0.294324	0.698027	0.567792
C	2	0.426881	0.687016	0.406059
C	3	0.576649	0.724512	0.337825
C	4	0.593426	0.774470	0.440435
C	5	0.464106	0.787869	0.602095
C	6	0.314732	0.749034	0.660748
C	7	0.939891	0.951934	0.029882
C	8	0.652699	0.951906	0.265444
C	9	0.989658	0.451926	0.113568
C	10	0.640172	0.548188	0.858558
C	11	0.294324	0.301973	0.567792
C	12	0.426881	0.312984	0.406059
C	13	0.576650	0.275488	0.337824
C	14	0.593426	0.225530	0.440435
C	15	0.464106	0.212131	0.602095
C	16	0.314732	0.250965	0.660748
C	17	0.939891	0.048066	0.029882
C	18	0.652699	0.048094	0.265444

```
x  C          19         0.989658   0.548074   0.113568   x
x  C          20         0.640172   0.451812   0.858558   x
x  C          21         0.586626   0.000000   0.926728   x
x  C          22         0.003962   0.000000   0.366152   x
x  C          23         0.662186   0.500000   0.192027   x
x  C          24         0.971435   0.500000   0.777447   x
x  N           1         0.689448   0.950951   0.035055   x
x  N           2         0.893724   0.549113   0.878633   x
x  N           3         0.689447   0.049049   0.035055   x
x  N           4         0.893724   0.450887   0.878633   x
x  N           5         0.049194   0.000000   0.139119   x
x  N           6         0.756318   0.000000   0.379632   x
x  N           7         0.915093   0.500000   0.220703   x
x  N           8         0.558420   0.500000   0.960724   x
x  F           1         0.412987   0.637508   0.313834   x
x  F           2         0.745725   0.810620   0.384853   x
x  F           3         0.190289   0.760959   0.820019   x
x  F           4         0.412988   0.362492   0.313834   x
x  F           5         0.745727   0.189380   0.384854   x
x  F           6         0.190287   0.239040   0.820018   x
x  I           1         0.096297   0.636398   0.692271   x
x  I           2         0.779621   0.705581   0.097575   x
x  I           3         0.530903   0.860153   0.785608   x
x  I           4         0.096298   0.363601   0.692271   x
x  I           5         0.779622   0.294419   0.097575   x
x  I           6         0.530904   0.139847   0.785608   x
xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
```