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Supporting information for article:

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Structural differences/similarities of diastereotopic groups in three new chiral phosphoramides

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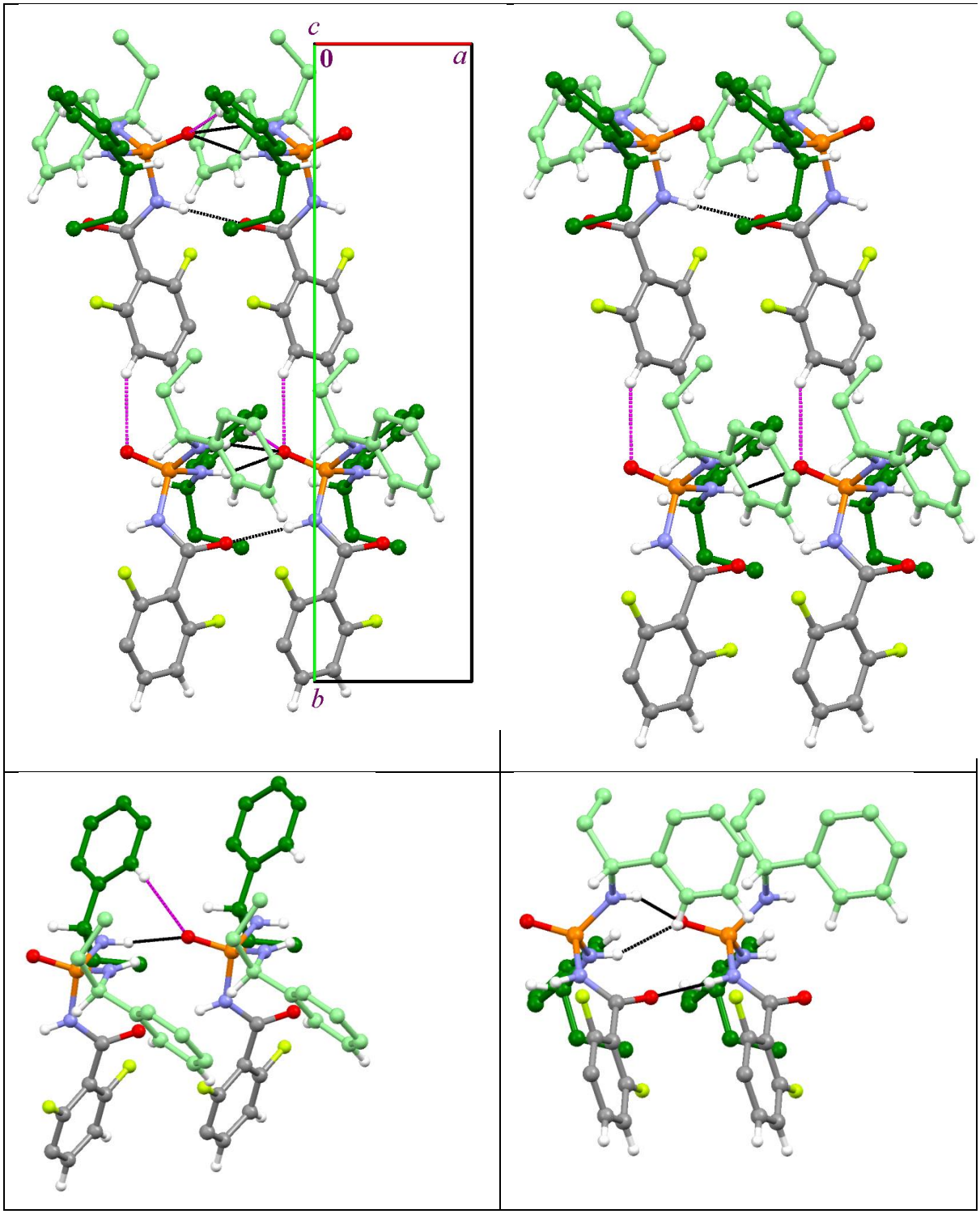

Figure S1 (Top-left) Partial part of crystal packing of structure (III) showing the hydrogen-bonded motifs constructed from N—H…O and C—H…O hydrogen bonds, including (top-right) $R_4^3(22)$, (bottom-left) $R_2^1(7)$ and (bottom-right) $R_2^2(10)$ and $R_2^1(6)$. The colours for fragments and dashed line are as the same as explained in the paper.

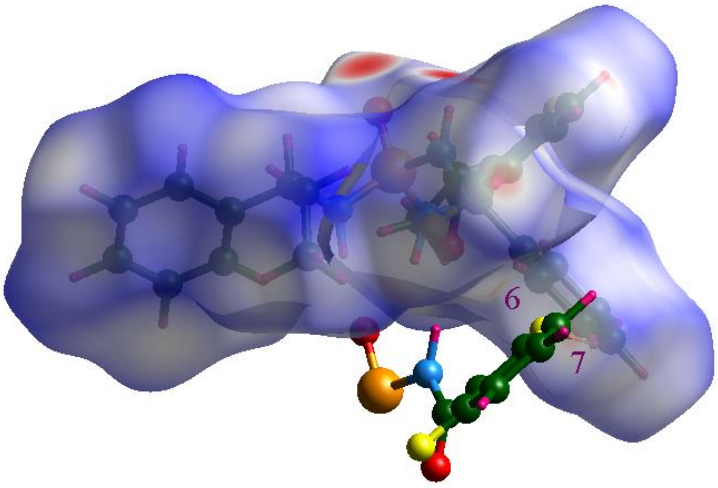

Figure S2 Labels 6 and 7 show F…O and F…H contacts in the structure (III). For the molecule outside the HS, only the fragment P(O)(NHC(O)$C_6H_3F_2$) is represented.

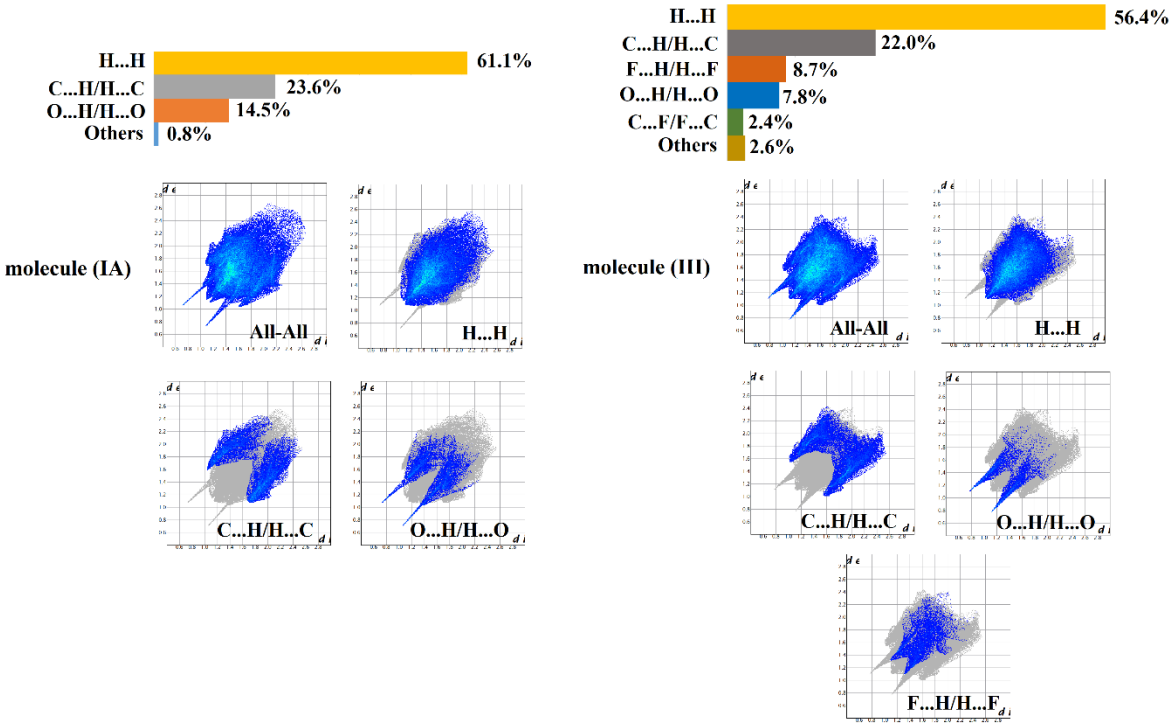

Figure S3 Two-dimensional fingerprint plots of molecules (I*A*) [left] and (III) [right].

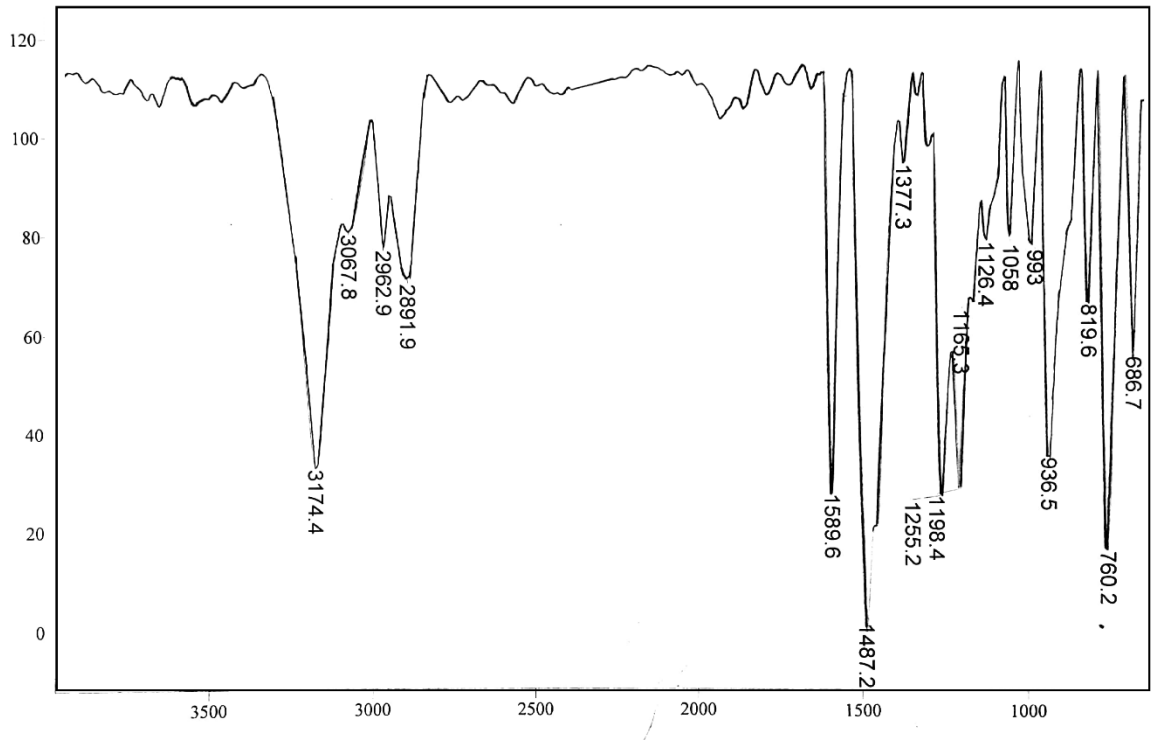

Figure S4 IR spectrum of (I).

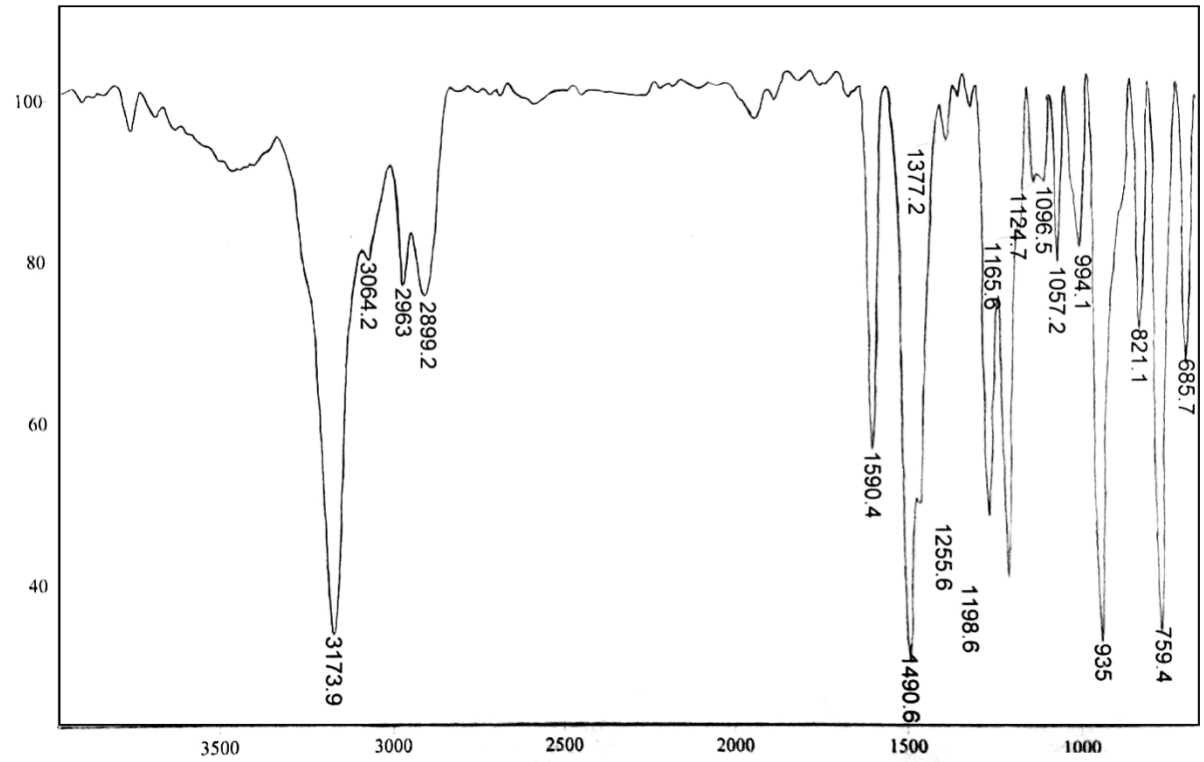

Figure S5 IR spectrum of (II).

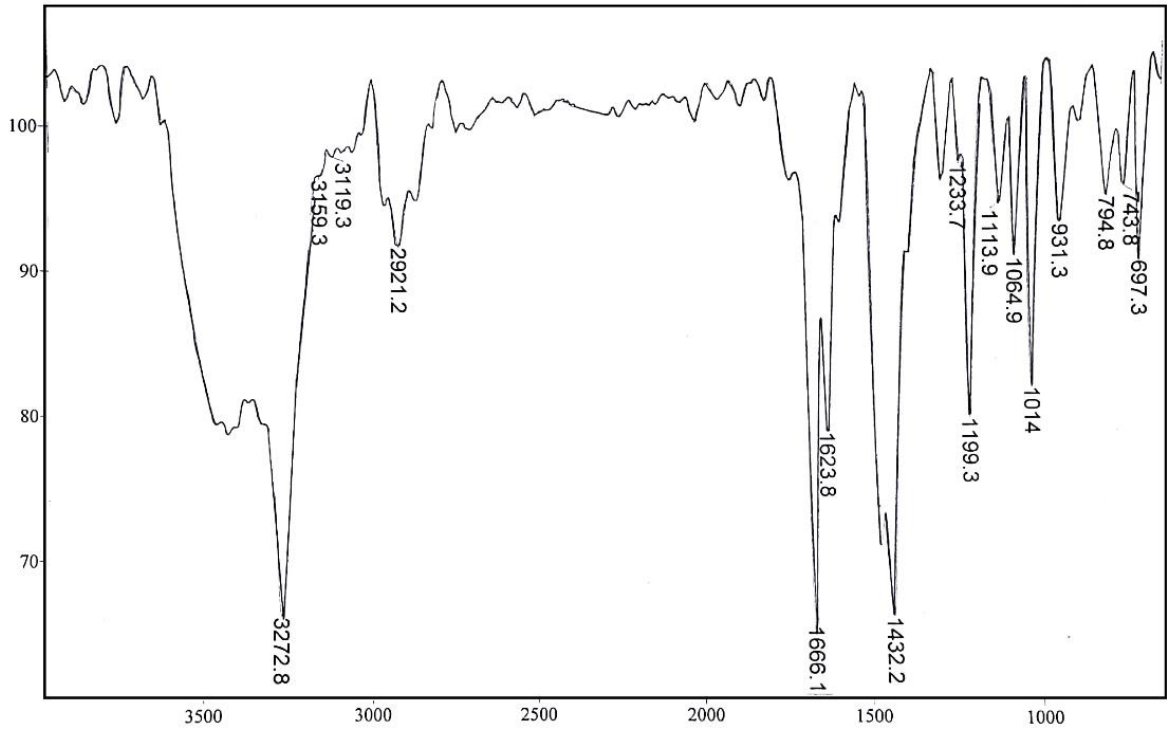

Figure S6 IR spectrum of (III).

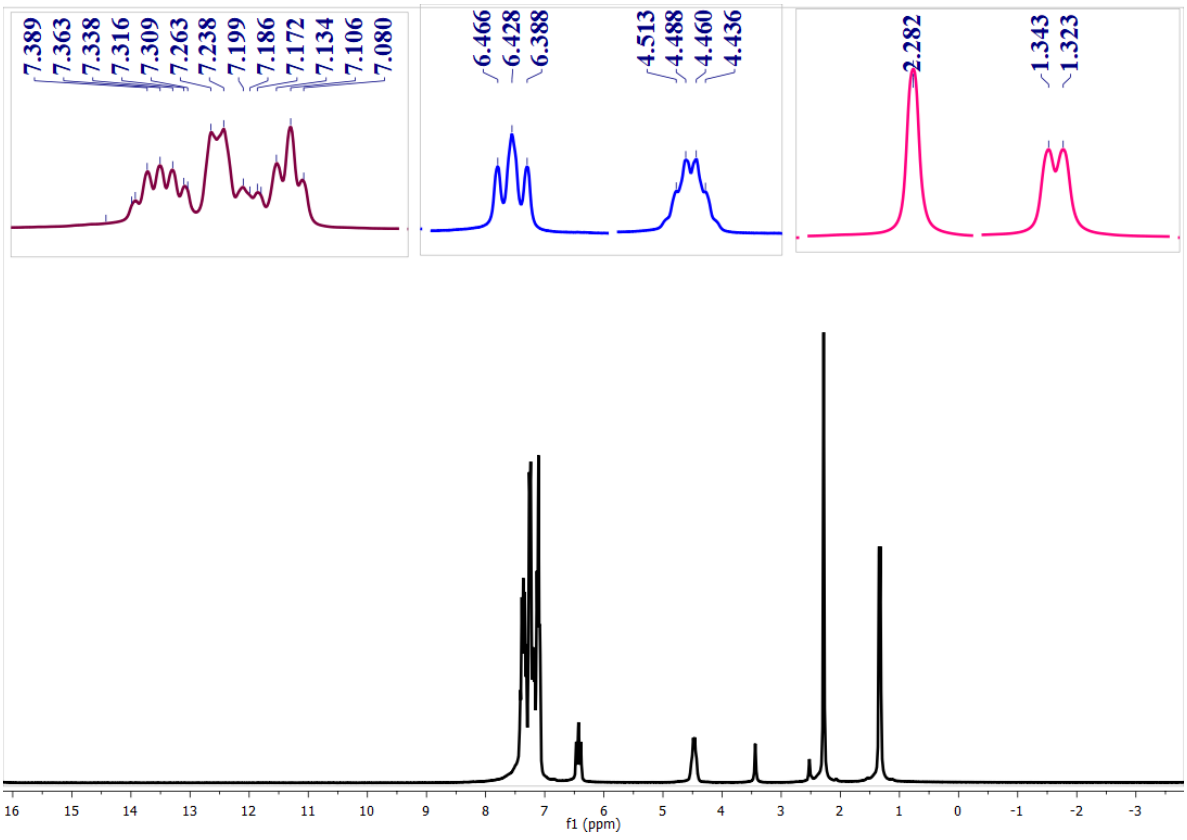

Figure S7 ^{1}H NMR spectrum of (I).

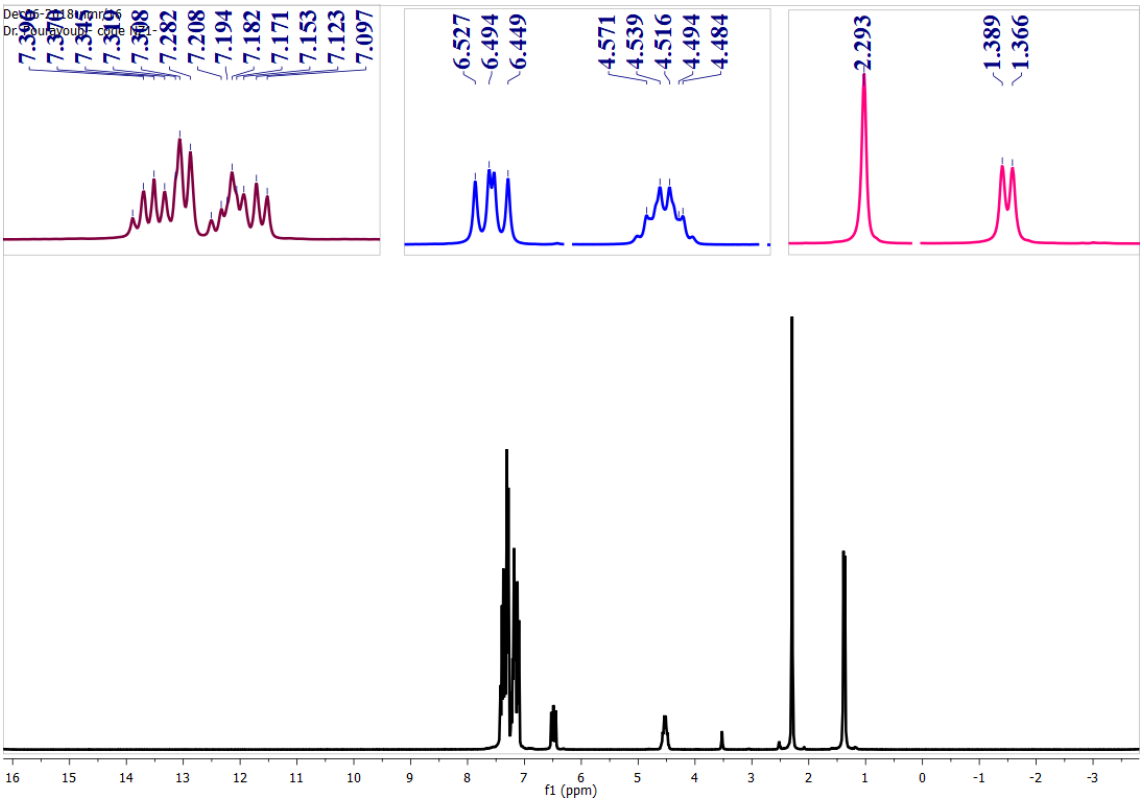

Figure S8 ^{1}H NMR spectrum of (II).

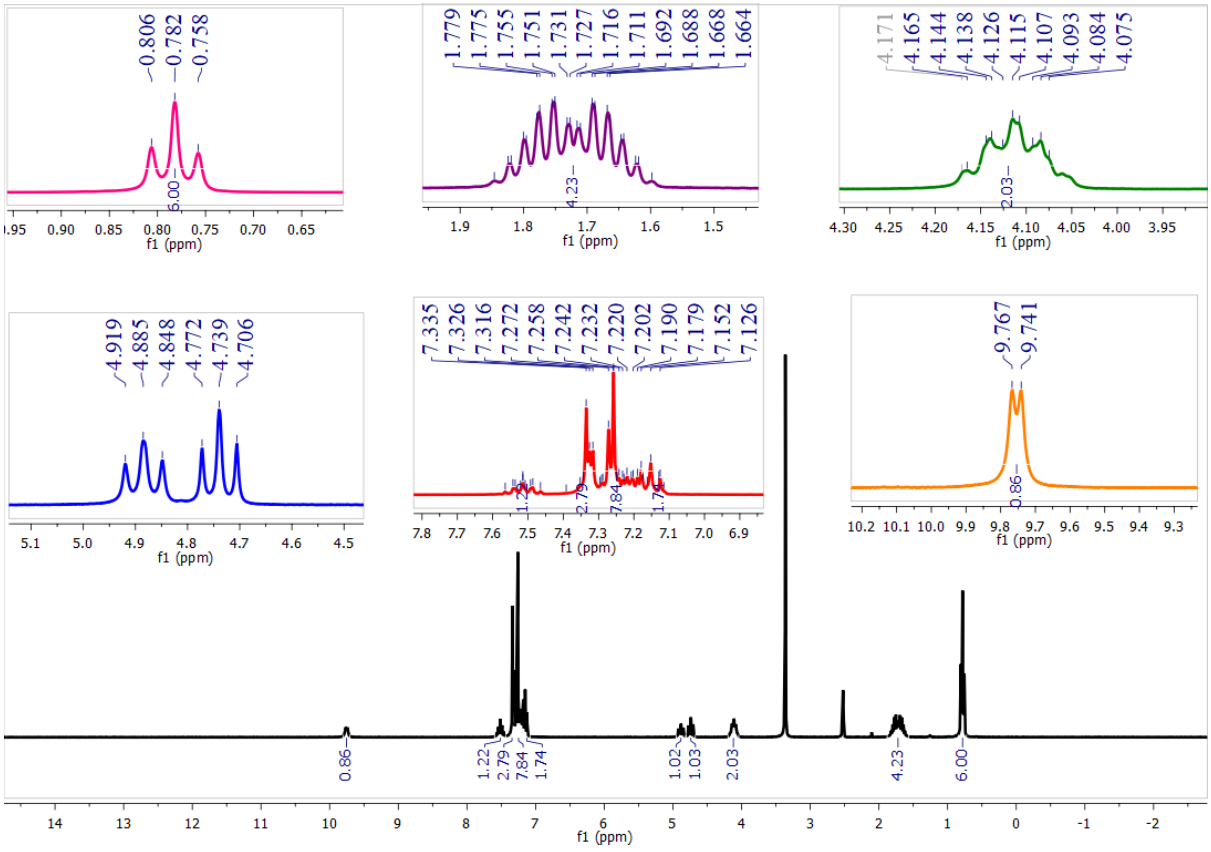

Figure S9 ^{1}H NMR spectrum of (III).

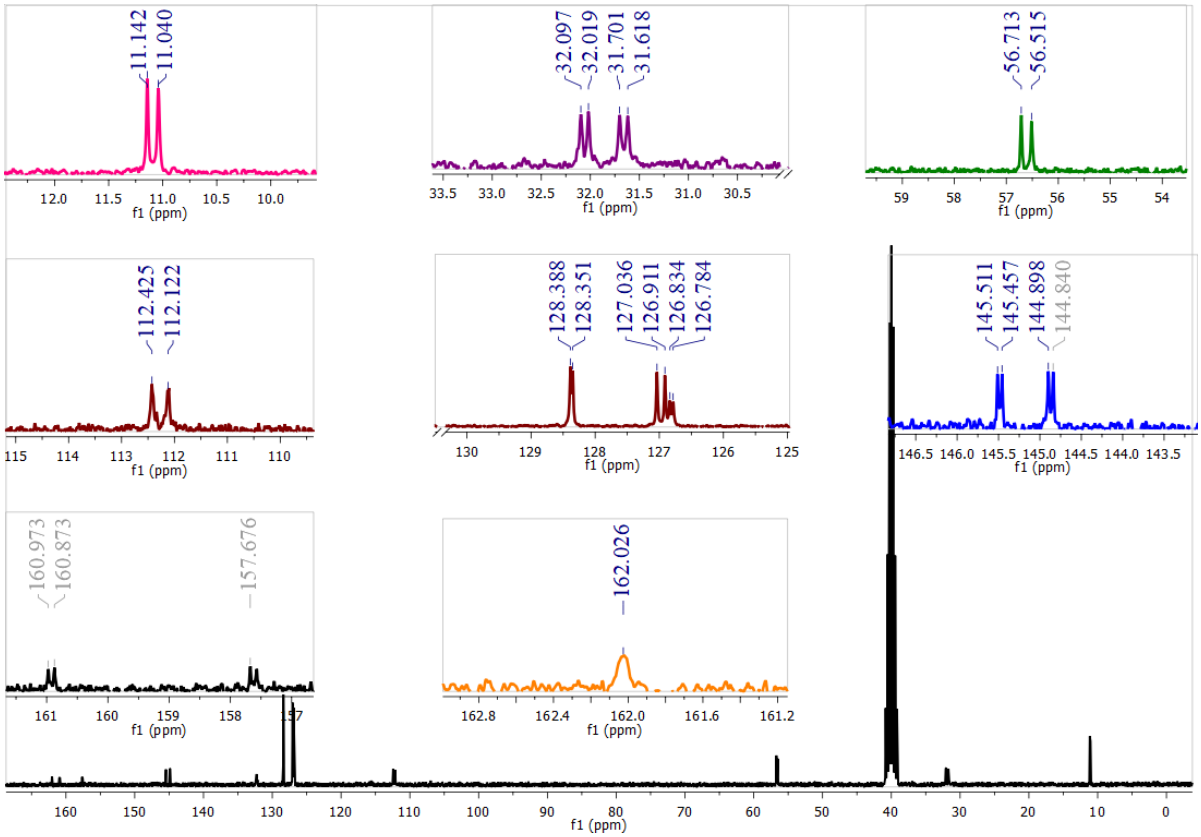

Figure S10 $^{13}C\{^{1}H\}$ NMR spectrum of (III).

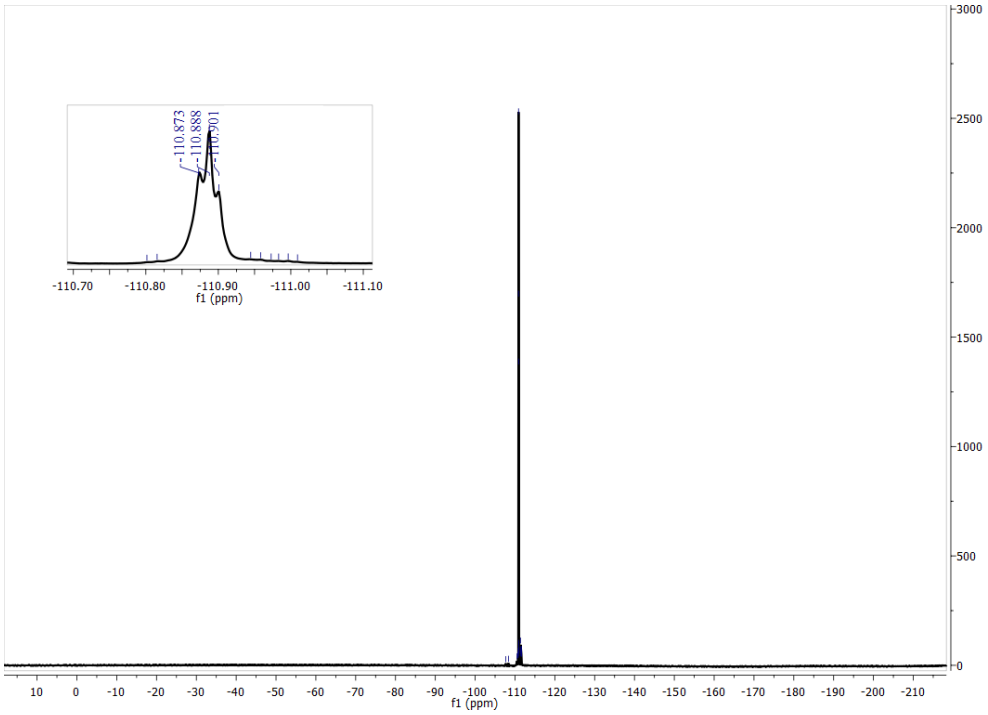

Figure S11 ^{19}F NMR spectrum of (III).

Table S1 Bond lengths of diastereotopic groups, and differences (Δ) in (I) and (II).

I*A*							
P1-O2	O2-C1	C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C1
1.5997(13)	1.390(2)	1.382(3)	1.390(3)	1.390(3)	1.378(4)	1.388(3)	1.386(3)
P1-O3	O3-C7	C7-C8	C8-C9	C9-C10	C10-C11	C11-C12	C12-C7
1.5870(14)	1.406(2)	1.385(3)	1.389(3)	1.386(3)	1.384(3)	1.391(3)	1.378(3)
Δ							
0.0127	–0.016	–0.003	0.001	0.004	–0.006	–0.003	0.008
I*B*							
P2-O5	O5-C22	C22-C23	C23-C24	C24-C25	C25-C26	C26-C27	C27-C22
1.5932(13)	1.408(2)	1.377(3)	1.390(3)	1.387(3)	1.377(3)	1.390(3)	1.385(3)
P2-O6	O6-C28	C28-C33	C33-C32	C32-C31	C31-C30	C30-C29	C29-C28
1.5930(14)	1.400(2)	1.380(3)	1.389(3)	1.383(3)	1.384(3)	1.386(3)	1.383(3)
Δ							
0.0002	0.008	–0.003	0.001	0.004	–0.007	0.004	0.002
II*A*							
P1-O2	O2-C1	C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C1
1.598(2)	1.395(4)	1.380(5)	1.392(5)	1.394(6)	1.377(6)	1.390(5)	1.383(5)
P1-O3	O3-C7	C7-C8	C8-C9	C9-C10	C10-C11	C11-C12	C12-C7
1.589(2)	1.404(4)	1.386(5)	1.388(5)	1.389(5)	1.381(5)	1.398(5)	1.378(5)
Δ							
0.009	–0.009	–0.006	0.004	0.005	–0.004	–0.008	0.005
II*B*							
P2-O5	O5-C22	C22-C23	C23-C24	C24-C25	C25-C26	C26-C27	C27-C22
1.591(2)	1.411(4)	1.376(5)	1.399(5)	1.381(6)	1.383(6)	1.391(5)	1.382(5)
P2-O6	O6-C28	C28-C33	C33-C32	C32-C31	C31-C30	C30-C29	C29-C28
1.596(2)	1.399(4)	1.382(5)	1.392(5)	1.383(6)	1.381(6)	1.388(5)	1.387(5)
Δ							
–0.005	0.012	–0.006	0.007	–0.002	0.002	0.003	–0.005

Table S2 Bond angles of diastereotopic groups, and differences (Δ) in (I) and (II).

I*A*									
O1-P1-O2	P1-O2-C1	O2-C1-C2	C1-C2-C3	C2-C3-C4	C3-C4-C5	C4-C5-C6	C5-C6-C1	C6-C1-C2	C6-C1-O2
115.72(8)	124.99(13)	123.81(18)	118.7(2)	120.5(2)	119.8(2)	120.4(2)	119.1(2)	121.46(19)	114.72(18)
O1-P1-O3	P1-O3-C7	O3-C7-C8	C7-C8-C9	C8-C9-C10	C9-C10-C11	C10-C11-C12	C11-C12-C7	C12-C7-C8	C12-C7-O3
116.43(8)	123.70(12)	120.00(17)	118.24(18)	120.86(19)	119.65(19)	120.45(19)	118.70(18)	122.09(18)	117.70(17)
Δ									
–0.71	1.29	3.81	0.46	–0.36	0.15	–0.05	0.4	–0.63	–2.98
I*B*									
O4-P2-O5	P2-O5-C22	O5-C22-C23	C22-C23-C24	C23-C24-C25	C24-C25-C26	C25-C26-C27	C26-C27-C22	C27-C22-C23	C27-C22-O5
115.13(8)	119.41(11)	118.76(18)	118.5(2)	120.4(2)	120.23(19)	120.2(2)	118.7(2)	122.05(18)	119.08(17)
O4-P2-O6	P2-O6-C28	O6-C28-C33	C28-C33-C32	C33-C32-C31	C32-C31-C30	C31-C30-C29	C30-C29-C28	C29-C28-C33	C29-C28-O6
115.88(8)	122.30(13)	122.79(17)	118.76(19)	120.7(2)	119.60(19)	120.50(19)	118.98(19)	121.49(18)	115.71(17)
Δ									
–0.75	–2.89	–4.03	–0.26	–0.3	0.63	–0.3	–0.28	0.56	3.37
II*A*									
O1-P1-O2	P1-O2-C1	O2-C1-C2	C1-C2-C3	C2-C3-C4	C3-C4-C5	C4-C5-C6	C5-C6-C1	C6-C1-C2	C6-C1-O2
115.68(13)	125.0(2)	123.6(3)	118.7(4)	120.3(4)	119.9(3)	120.5(4)	118.9(4)	121.7(3)	114.6(3)
O1-P1-O3	P1-O3-C7	O3-C7-C8	C7-C8-C9	C8-C9-C10	C9-C10-C11	C10-C11-C12	C11-C12-C7	C12-C7-C8	C12-C7-O3
116.33(13)	123.7(2)	120.0(3)	118.3(3)	120.9(3)	119.6(3)	120.6(3)	118.5(3)	122.1(3)	117.7(3)
Δ									
–0.65	1.3	3.6	0.4	–0.6	0.3	–0.1	0.4	–0.4	–3.1
II*B*									
O4-P2-O5	P2-O5-C22	O5-C22-C23	C22-C23-C24	C23-C24-C25	C24-C25-C26	C25-C26-C27	C26-C27-C22	C27-C22-C23	C27-C22-O5
115.33(13)	119.4(2)	118.5(3)	118.4(4)	120.3(4)	120.3(3)	120.2(4)	118.6(3)	122.2(3)	119.1(3)
O4-P2-O6	P2-O6-C28	O6-C28-C33	C28-C33-C32	C33-C32-C31	C32-C31-C30	C31-30-C29	C30-C29-C28	C29-C28-C33	C29-C28-O6
115.90(13)	122.1(2)	122.9(3)	118.5(3)	120.9(3)	119.5(3)	120.8(3)	118.7(3)	121.6(3)	115.5(3)
Δ									
–0.57	–2.7	–4.4	–0.1	–0.6	0.8	–0.6	–0.1	0.6	3.6

Table S3 Details of conformational analysis of diastereotopic groups, including "torsion angle" (TA) and associated "conformation" (C) for structures (I) and (II).

	TA	**C**	**TA**	**C**	**TA**	**C**	**TA**	**C**
I*A*	P1-O2-C1-C2 (20.12)	+*sp*	P1-O2-C1-C6 (–161.36)	–*ap*	P1-O3-C7-C8 (–71.14)	–*sc*	P1-O3-C7-C12 (113.96)	+*ac*
I*B*	P2-O5-C22-C23 (92.40)	+*ac*	P2-O5-C22-C27 (–91.25)	–*ac*	P2-O6-C28-C33 (–36.24)	–*sc*	P2-O6-C28-C29 (144.97)	+*ac*
II*A*	P1-O2-C1-C2 (–20.58)	–*sp*	P1-O2-C1-C6 (161.15)	+*ap*	P1-O3-C7-C8 (71.15)	+*sc*	P1-O3-C7-C12 (–113.91)	–*ac*
II*B*	P2-O5-C22-C23 (–92.26)	–*ac*	P2-O5-C22-C27 (90.97)	+*ac*	P2-O6-C28-C33 (36.12)	+*sc*	P2-O6-C28-C29 (–144.88)	–*ac*

Table S4 Bond lengths of diastereotopic groups, and differences (Δ) for (III).

P1-N14	N14-C15	C15-C22	C22-C23	C15-C16	C16-C21	C21-C20	C20-C19	C19-C18	C18-C17	C17-C16
1.6221(16)	1.471(2)	1.536(3)	1.519(3)	1.532(3)	1.395(3)	1.385(3)	1.384(4)	1.380(3)	1.396(3)	1.387(3)
P1-N24	N24-C25	C25-C32	C32-C33	C25-C26	C26-C31	C31-C30	C30-C29	C29-C28	C28-C27	C27-C26
1.6173(16)	1.475(2)	1.539(3)	1.526(3)	1.529(3)	1.396(3)	1.384(3)	1.380(3)	1.381(3)	1.390(3)	1.388(3)
Δ										
0.0048	–0.004	–0.003	–0.007	0.003	–0.001	0.001	0.004	–0.001	0.006	–0.001

Table S5 Bond angles of diastereotopic groups, and differences (Δ) for (III).

P1-N14-C15	N14-C15-C22	C15-C22-C23	N14-C15-C16	C22-C15-C16	C15-C16-C21	C16-C21-C20
123.74(13)	113.06(16)	113.66(17)	111.04(16)	111.22(16)	118.77(19)	120.9(2)
P1-N24-C25	N24-C25-C32	C25-C32-C33	N24-C25-C26	C32-C25-C26	C25-C26-C31	C26-C31-C30
122.74(13)	111.00(16)	114.71(18)	110.68(15)	115.55(16)	122.65(18)	120.9(2)
Δ						
1	2.06	–1.05	0.36	–4.33	–3.88	0
C21-C20-C19	C20-C19-C18	C19-C18-C17	C18-C17-C16	C17-C16-C21	C17-C16-C15	
120.3(2)	119.4(2)	120.4(2)	120.60(19)	118.40(19)	122.81(17)	
C31-C30-C29	C30-C29-C28	C29-C28-C27	C28-C27-C26	C27-C26-C31	C27-C26-C25	
120.6(2)	119.3(2)	120.1(2)	121.35(19)	117.72(19)	119.53(17)	
Δ						
–0.3	0.1	0.3	–0.75	0.68	3.28	

Table S6 Distance between the rings (Å) of the title compounds (I), (II) and (III).

I*A*	Ring (C1-C6)	Ring (C7-C12)	Ring (C15-C20)
Ring (C1-C6)	-	7.7435 (12)	7.3170 (13)
Ring (C7-C12)	7.7435 (12)	-	4.5668 (12)
Ring (C15-C20)	7.3170 (13)	4.5668 (12)	-
I*B*	Ring (C22-C27)	Ring (C28-C33)	Ring (C36-C41)
Ring (C22-C27)	-	7.6911 (12)	3.7519 (12)
Ring (C28-C33)	7.6911 (12)	-	7.8664 (12)
Ring (C36-C41)	3.7519 (12)	7.8664 (12)	-
II*A*	Ring (C1-C6)	Ring (C7-C12)	Ring (C15-C20)
Ring (C1-C6)	-	7.744 (2)	4.567 (2)
Ring (C7-C12)	7.744 (2)	-	7.317 (2)
Ring (C15-C20)	4.567 (2)	7.317 (2)	-
II*B*	Ring (C22-C27)	Ring (C28-C33)	Ring (C36-C41)
Ring (C22-C27)	-	7.692 (2)	7.866 (2)
Ring (C28-C33)	7.692 (2)	-	3.750 (2)
Ring (C36-C41)	7.866 (2)	3.750 (2)	-
(**III**)	Ring (C26-C31)	Ring (C6-C11)	Ring (C16-C21)
Ring (C26-C31)	-	7.2432 (12)	9.3429 (12)
Ring (C6-C11)	7.2432 (12)	-	8.9331 (13)
Ring (C16-C21)	9.3429 (12)	8.9331 (13)	-

Table S7 Contribution of close contacts in fingerprint plots of (I), (II) and (III).

	I*A* (%)	**I*B* (%)**	**II*A* (%)**	**II*B* (%)**	**III (%)**
H…H	61.1	60.2	61.1	60.3	56.4
C…H/H…C	23.6	24.1	23.6	24.0	22.0
O…H/H…O	14.5	15.2	14.5	15.2	7.8
F…H/H…F	-	-	-	-	8.7
C…F/F…C	-	-	-	-	2.4
Others	0.8[a]	0.5[b]	0.8[a]	0.5[b]	2.6[c]

[a](O…O) + (C…O/O…C) + (C…C).

[b](O…O).

[c](F…O/O…F) + (O…C/C…O) + (N…H/H…N) + (C…C).