Electronic Supplementary Material (ESI) for Dalton Transactions.

Electronic Supplementary Information for:

Synthesis and unique reversible splitting of 14-membered cyclic aminomethylphosphines on to 7-membered heterocycles.

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X-Ray Crystallography for 2a.

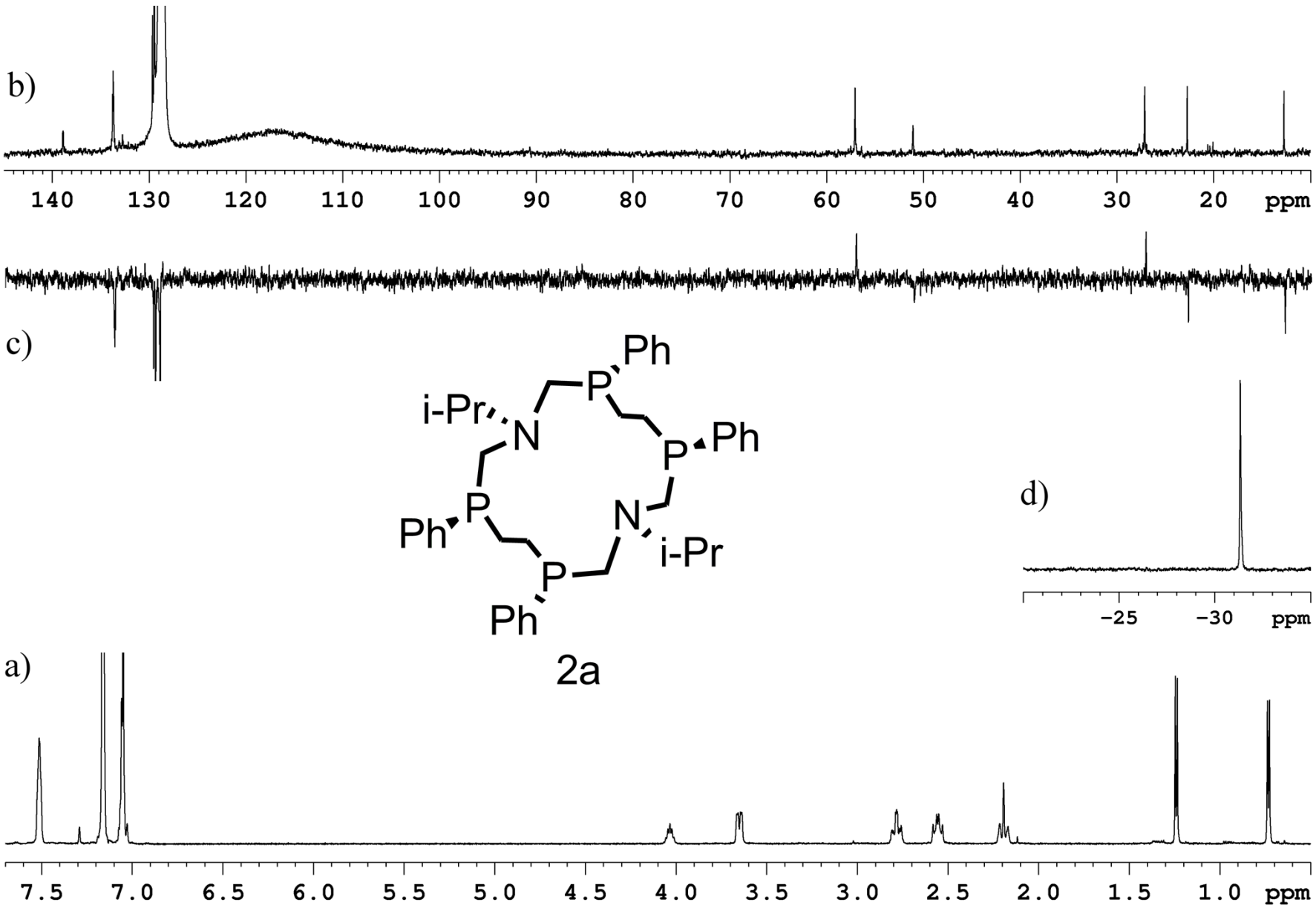


Figure S1. 1D ^{1}H (a), $^{13}C\{^{1}H\}$ (b), ^{13}C DEPT (c), and $^{31}P\{^{1}H\}$ (d) NMR spectra of **2a** in C_6D_6 at T = 303 K.

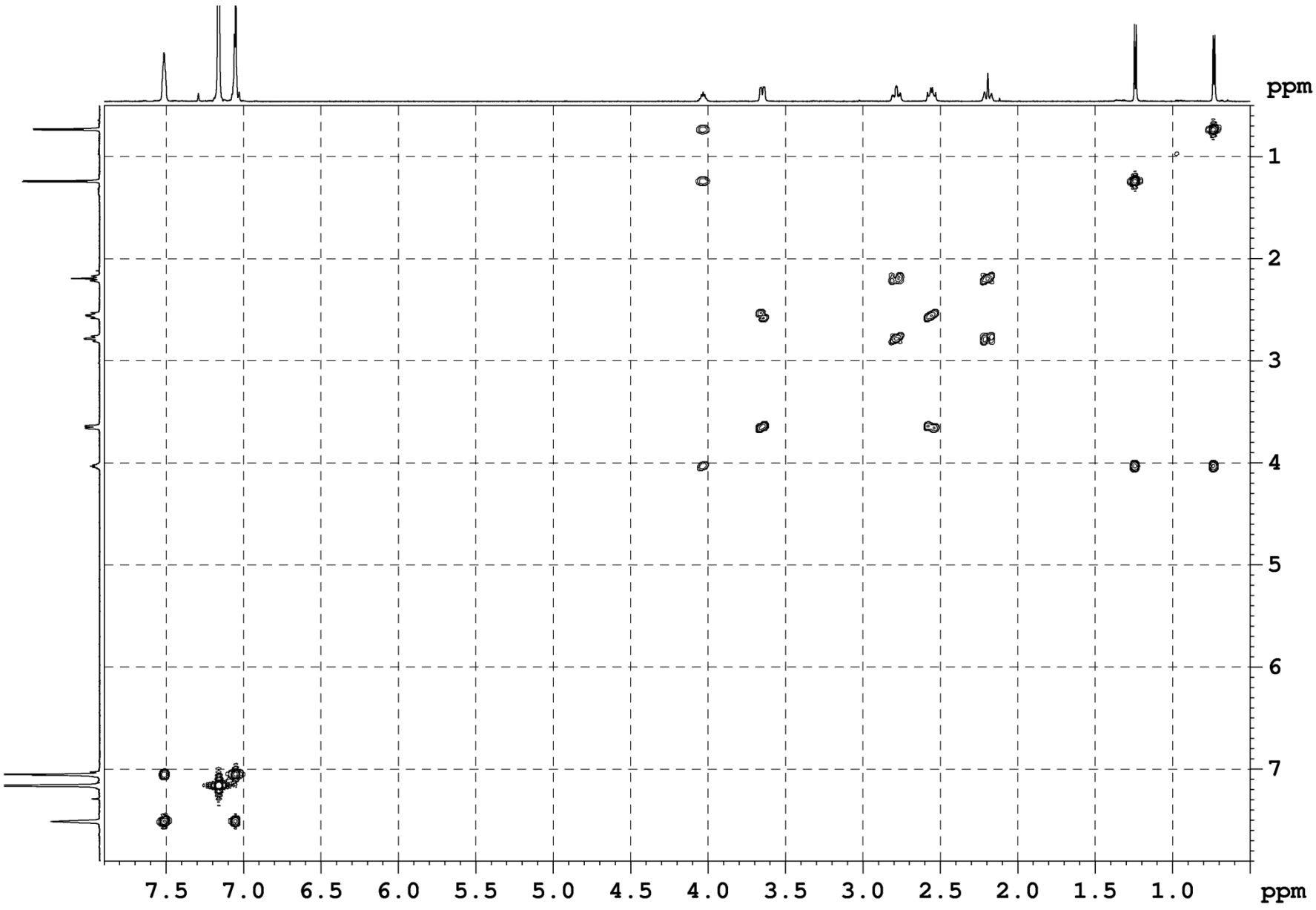


Figure S2. 2D ^{1}H-^{1}H COSY NMR spectra of **2a** in C_6D_6 at T = 303 K.

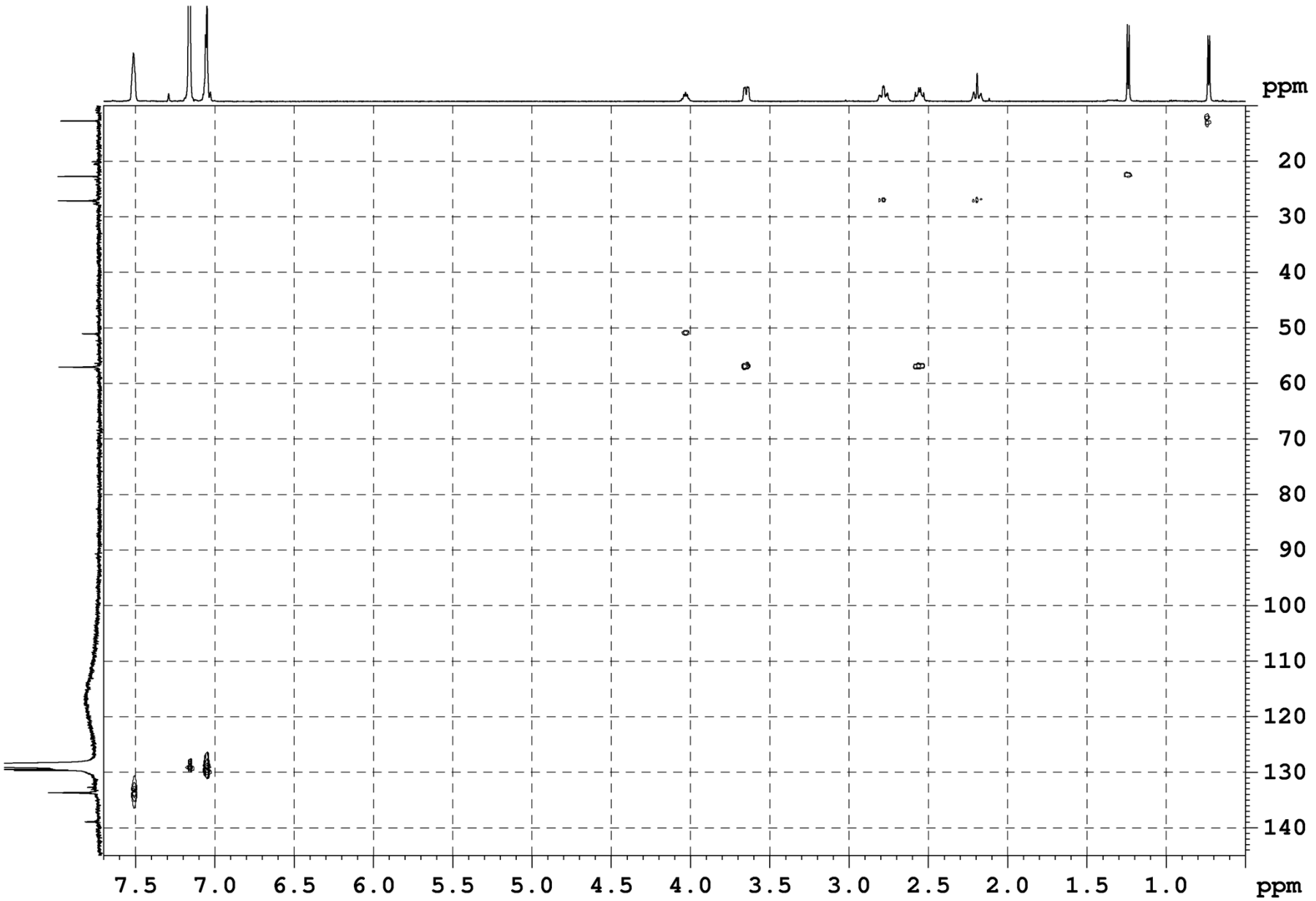


Figure S3. 2D ^{1}H-^{13}C HSQC NMR spectra of **2a** in C_6D_6 at T = 303 K.

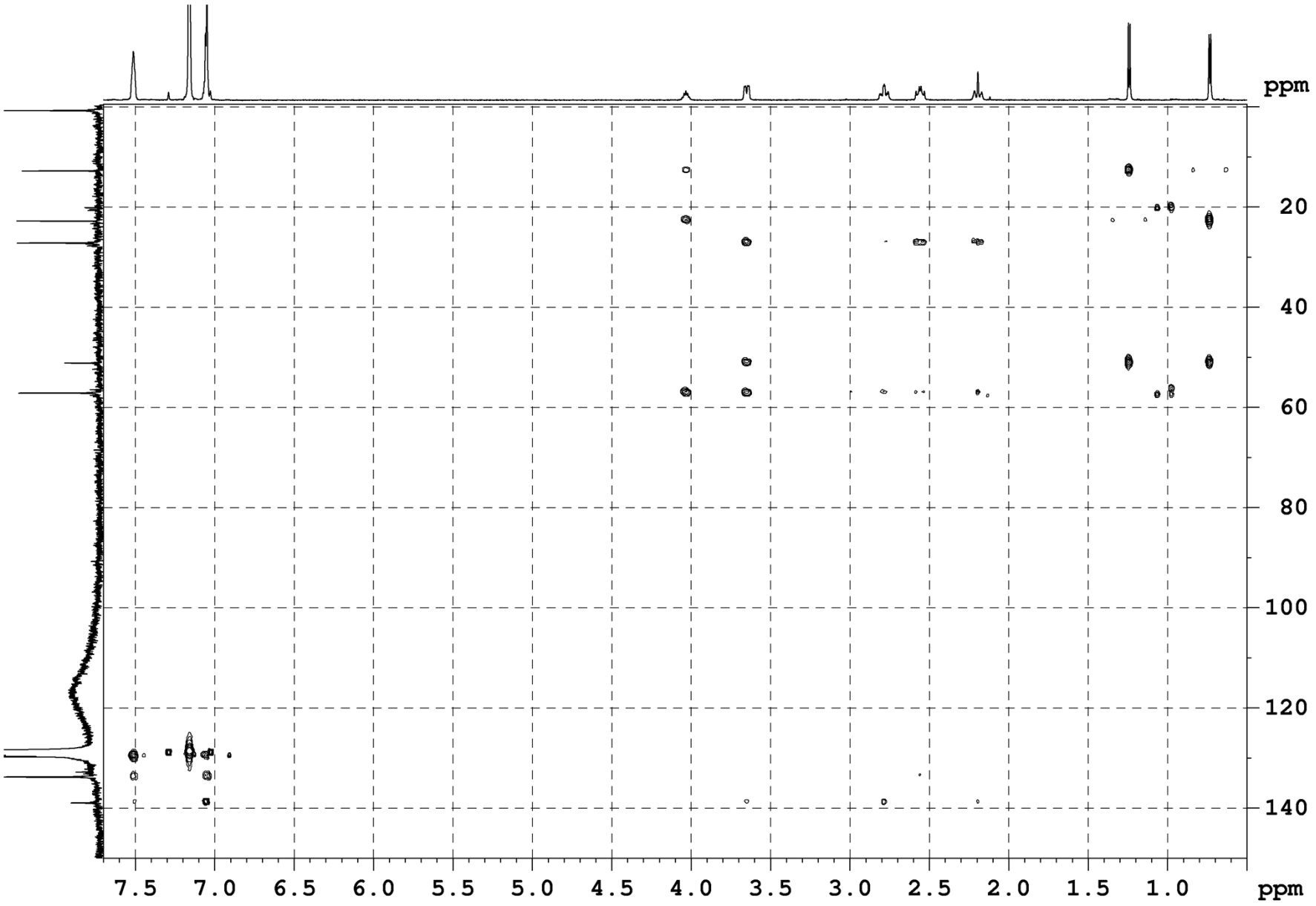


Figure S4. 2D ^{1}H-^{13}C HMBC NMR spectra of **2a** in C_6D_6 at T = 303 K.

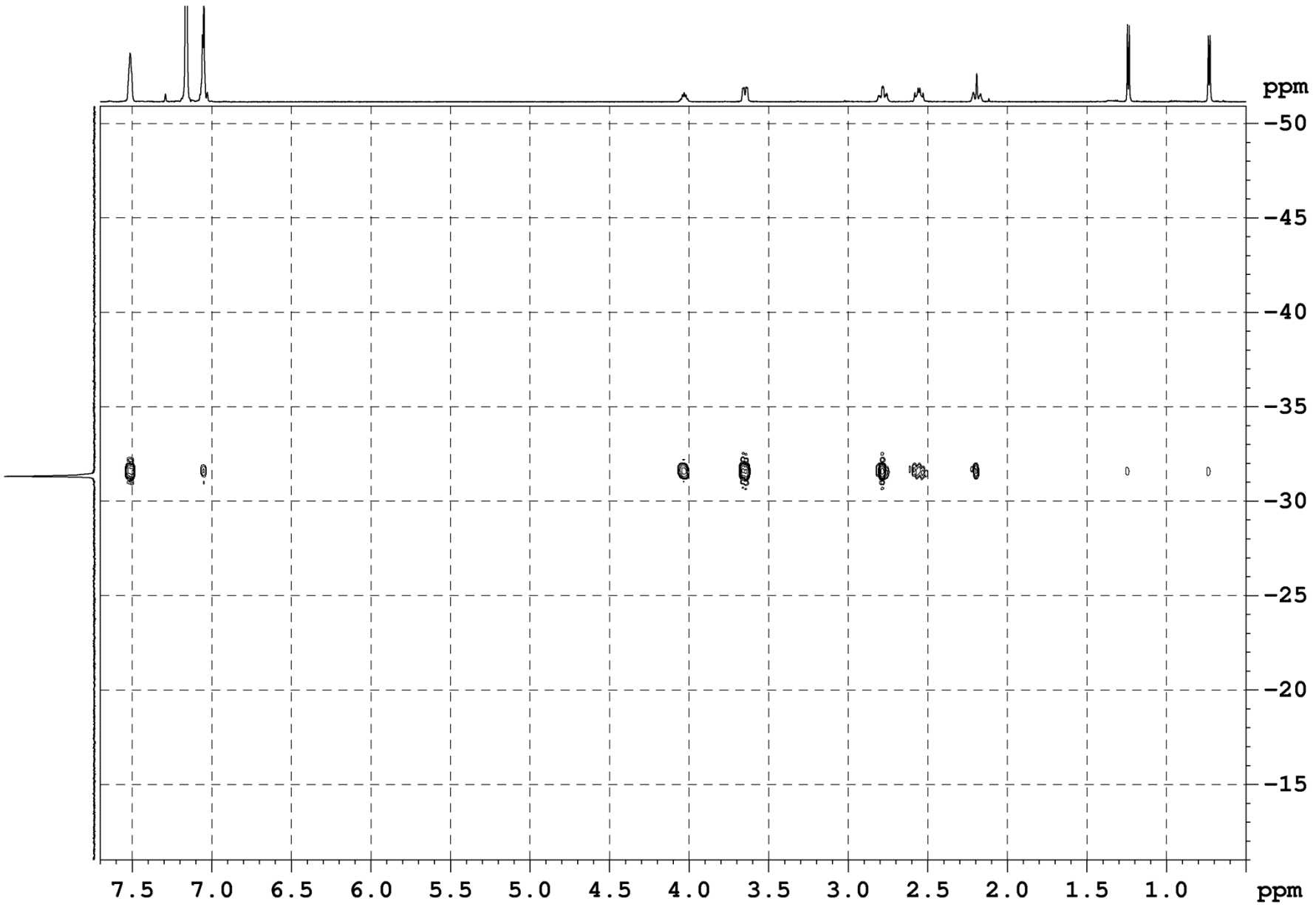


Figure S5. 2D ^{1}H-^{31}P HMBC NMR spectra of **2a** in C_6D_6 at T = 303 K.

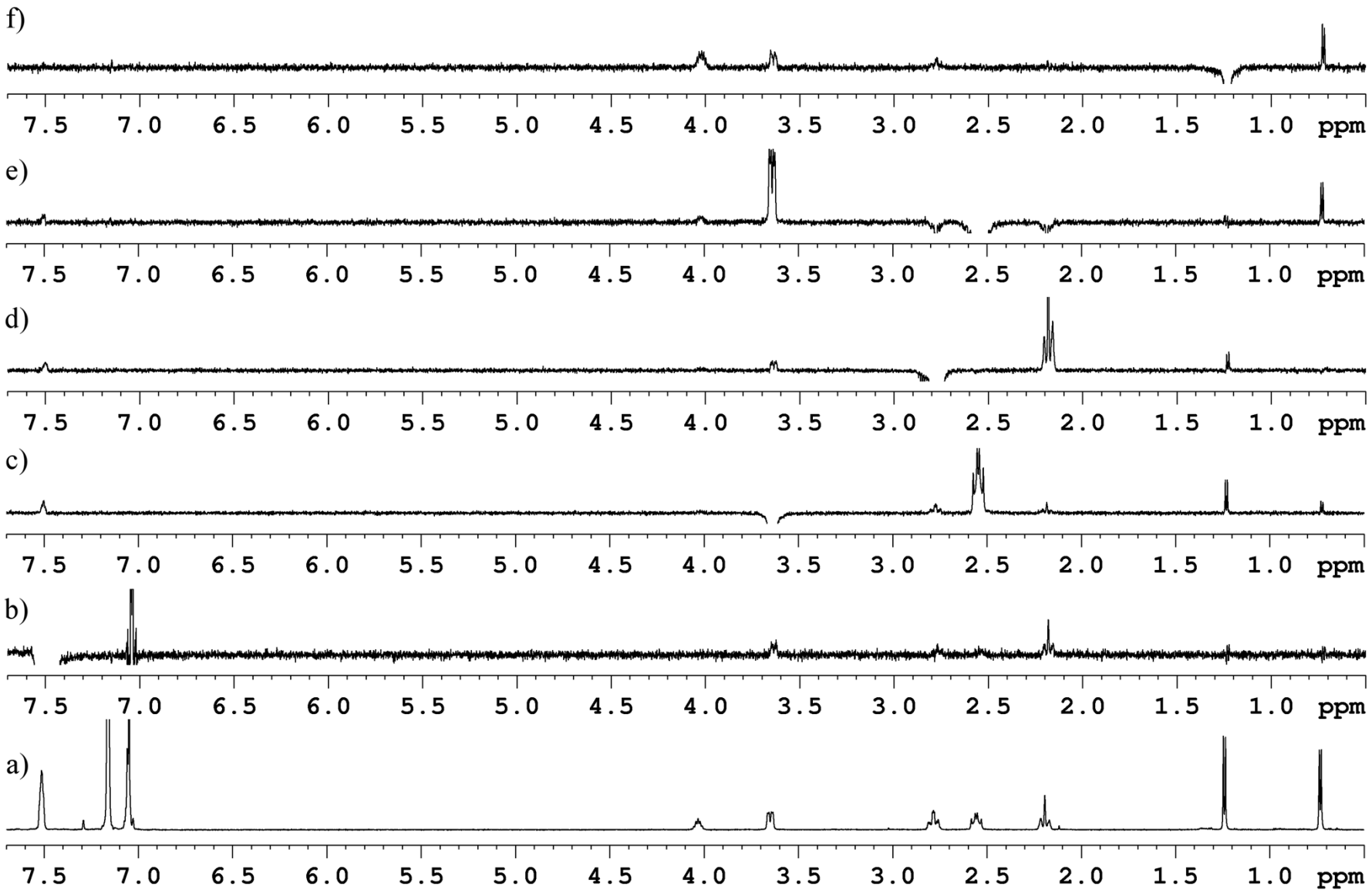


Figure S6. 1D ^{1}H (a) and 1D NOESY (b-f) NMR spectra of **2a** in C_6D_6 at T = 303 K.

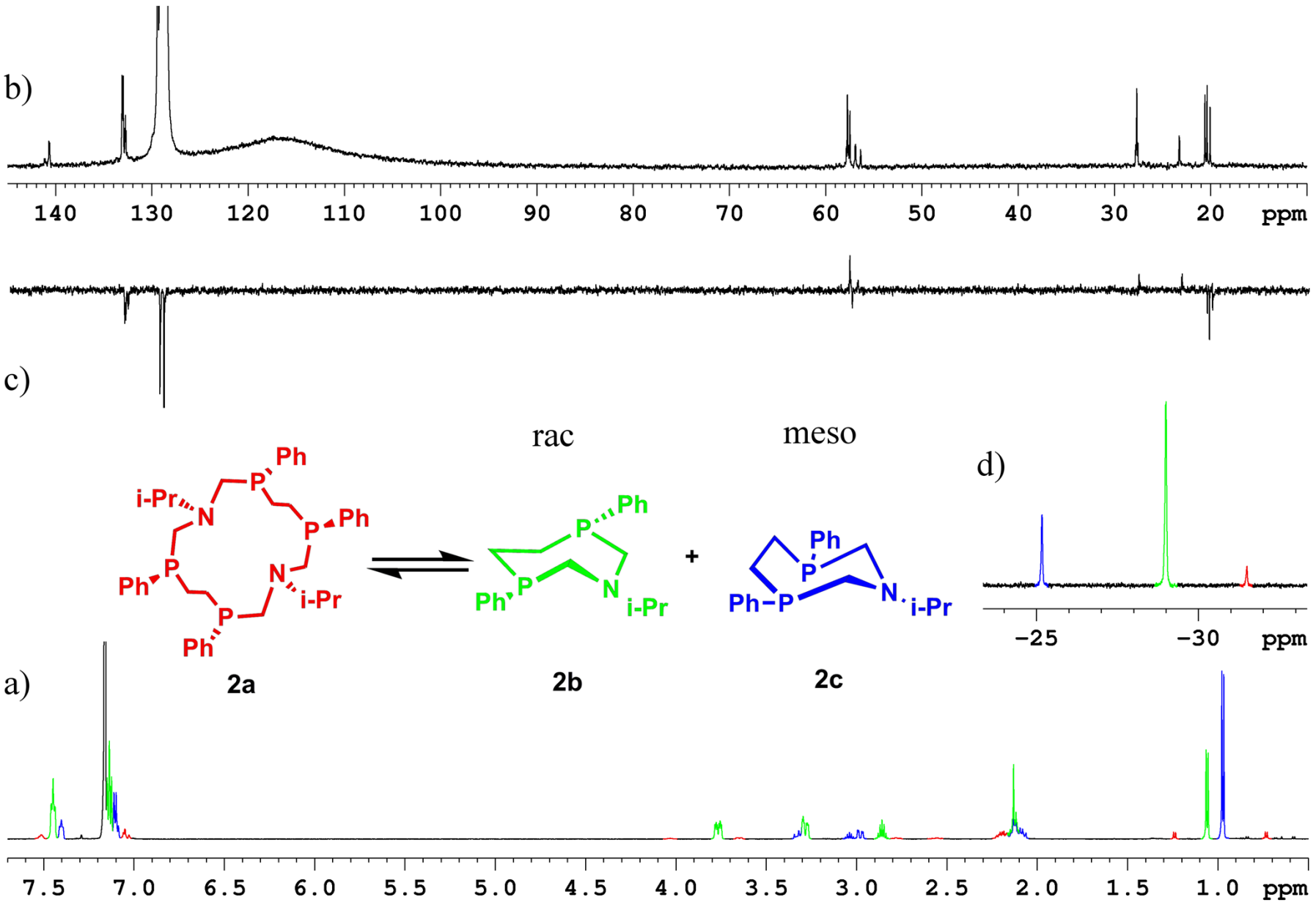


Figure S7. 1D ^{1}H (a), $^{13}C\{^{1}H\}$ (b), ^{13}C DEPT (c), and $^{31}P\{^{1}H\}$ (d) NMR spectra of **2a, 2b**, **2c** in C_6D_6 at T = 303 K after ca. 14 days.

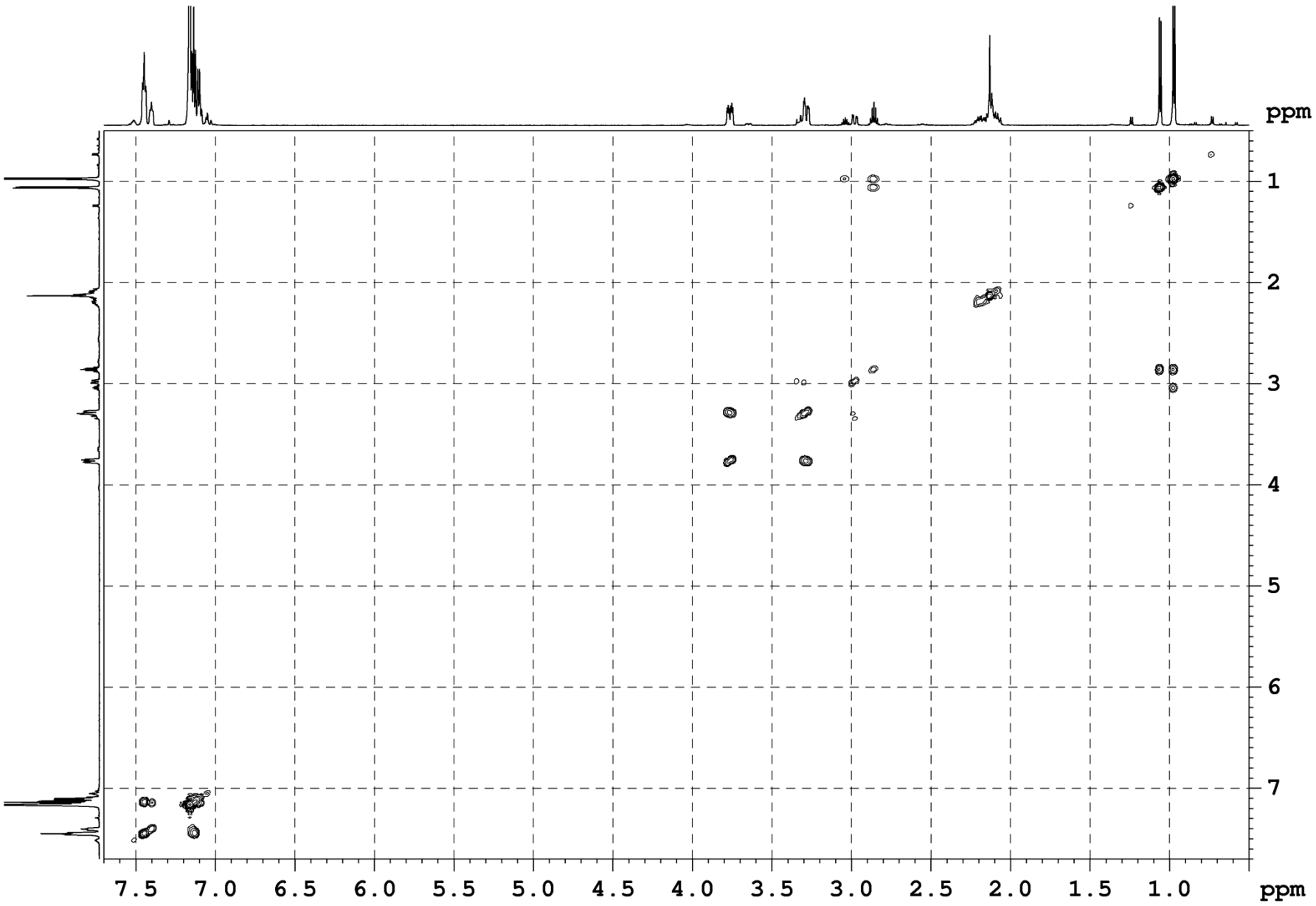


Figure S8. 2D ^{1}H-^{1}H COSY NMR spectra of **2a, 2b**, **2c** in C_6D_6 at T = 303 K after ca. 14 days.

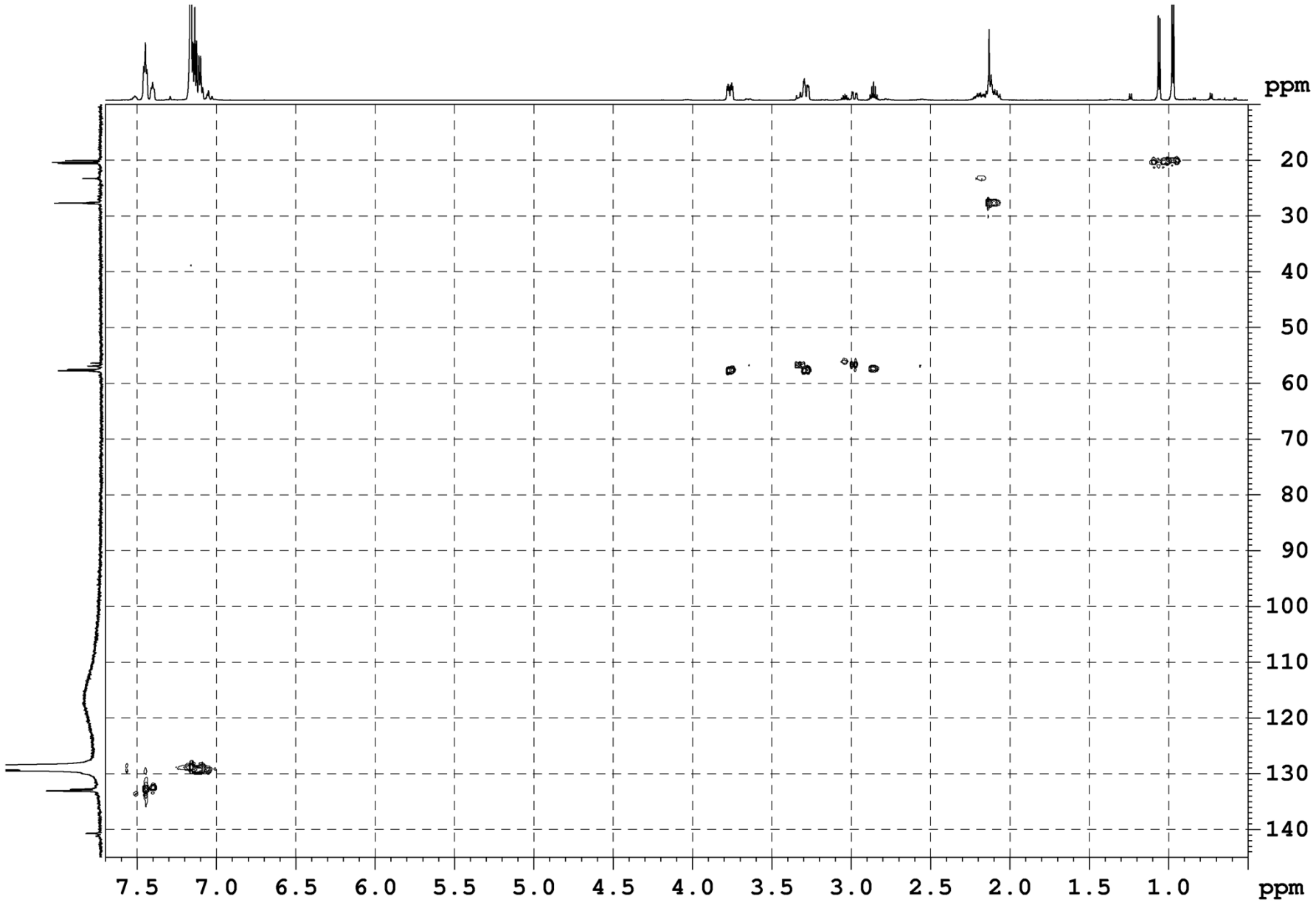


Figure S9. 2D ^{1}H-^{13}C HSQC NMR spectra of **2a, 2b**, **2c** in C_6D_6 at T = 303 K after ca. 14 days.

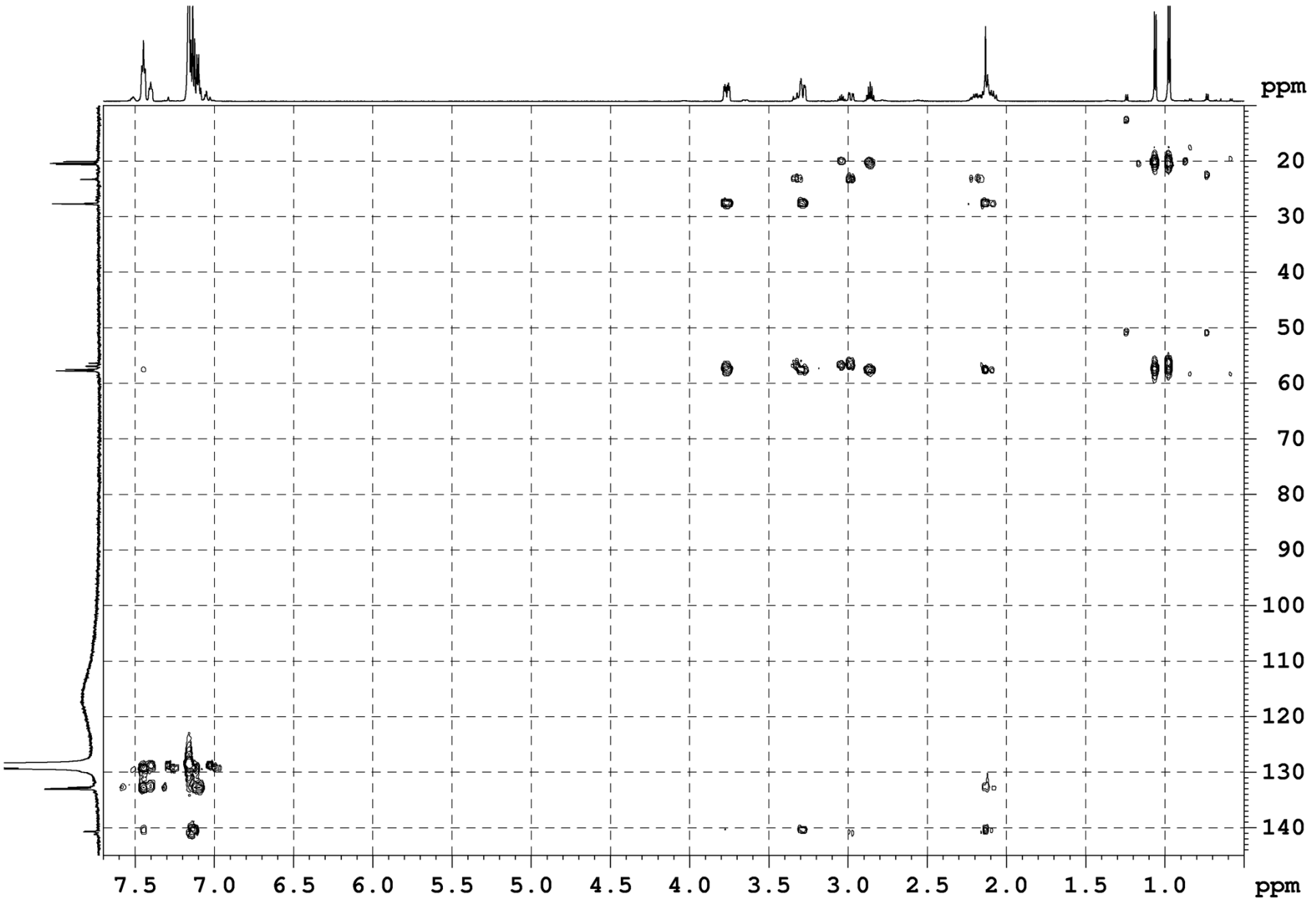


Figure S10. 2D ^{1}H-^{13}C HMBC NMR spectra of **2a, 2b**, **2c** in C_6D_6 at T = 303 K after ca. 14 days.

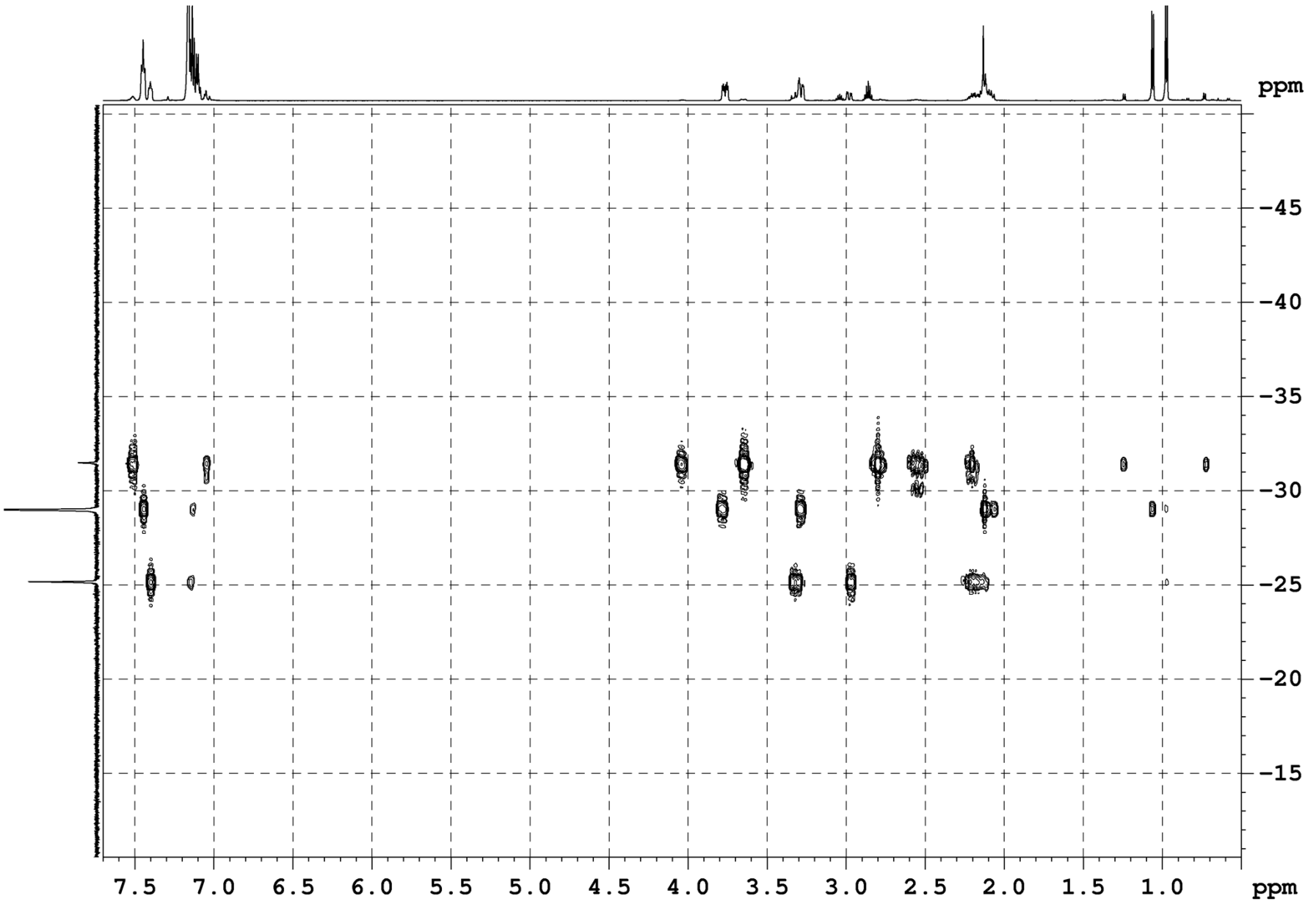


Figure S11. 2D ^{1}H-^{31}P HMBC NMR spectra of **2a, 2b**, **2c** in C_6D_6 at T = 303 K after ca. 14 days.

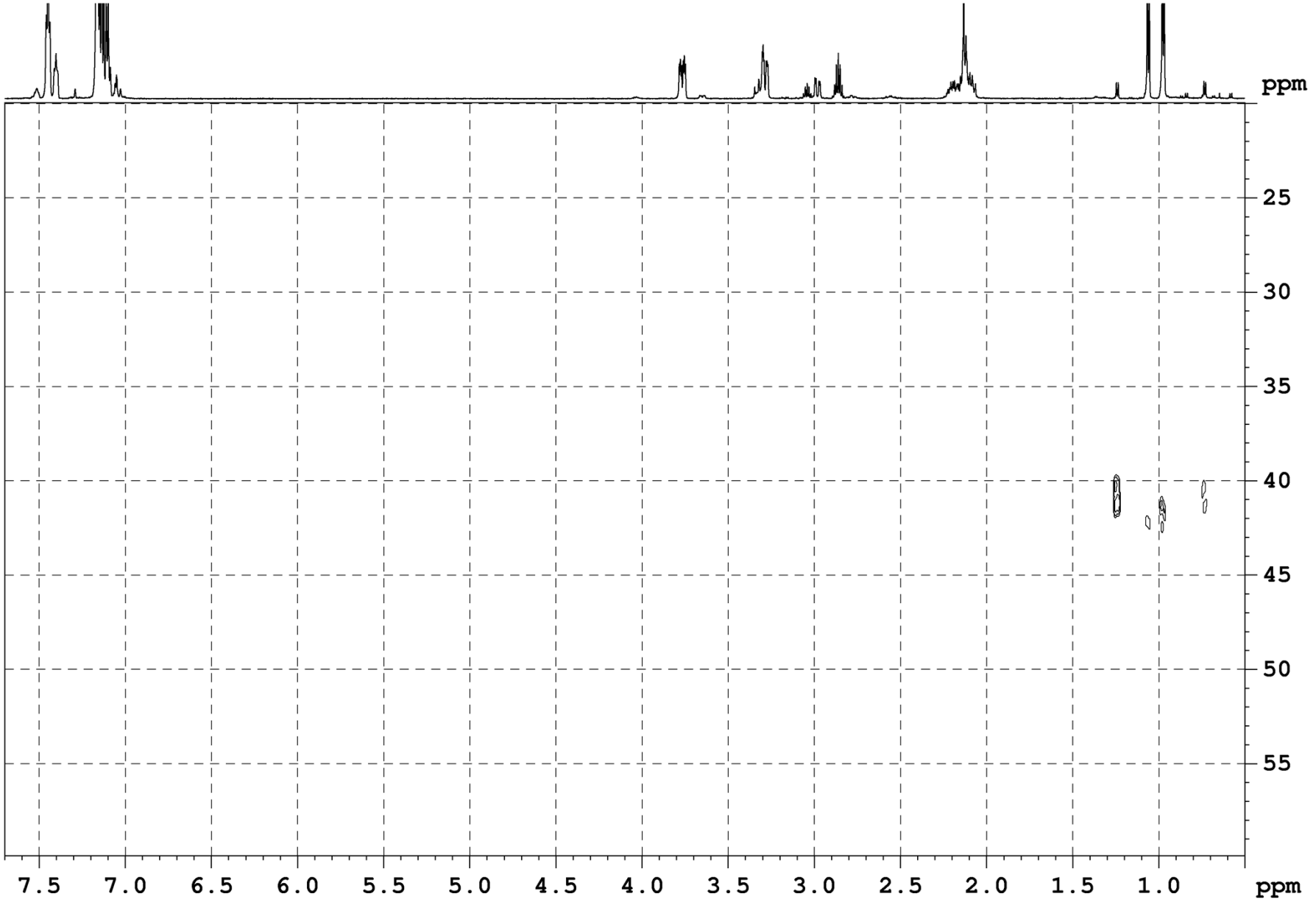


Figure S12. 2D ^{1}H-^{15}N HMBC NMR spectra of **2a, 2b**, **2c** in C_6D_6 at T = 303 K after ca. 14 days.

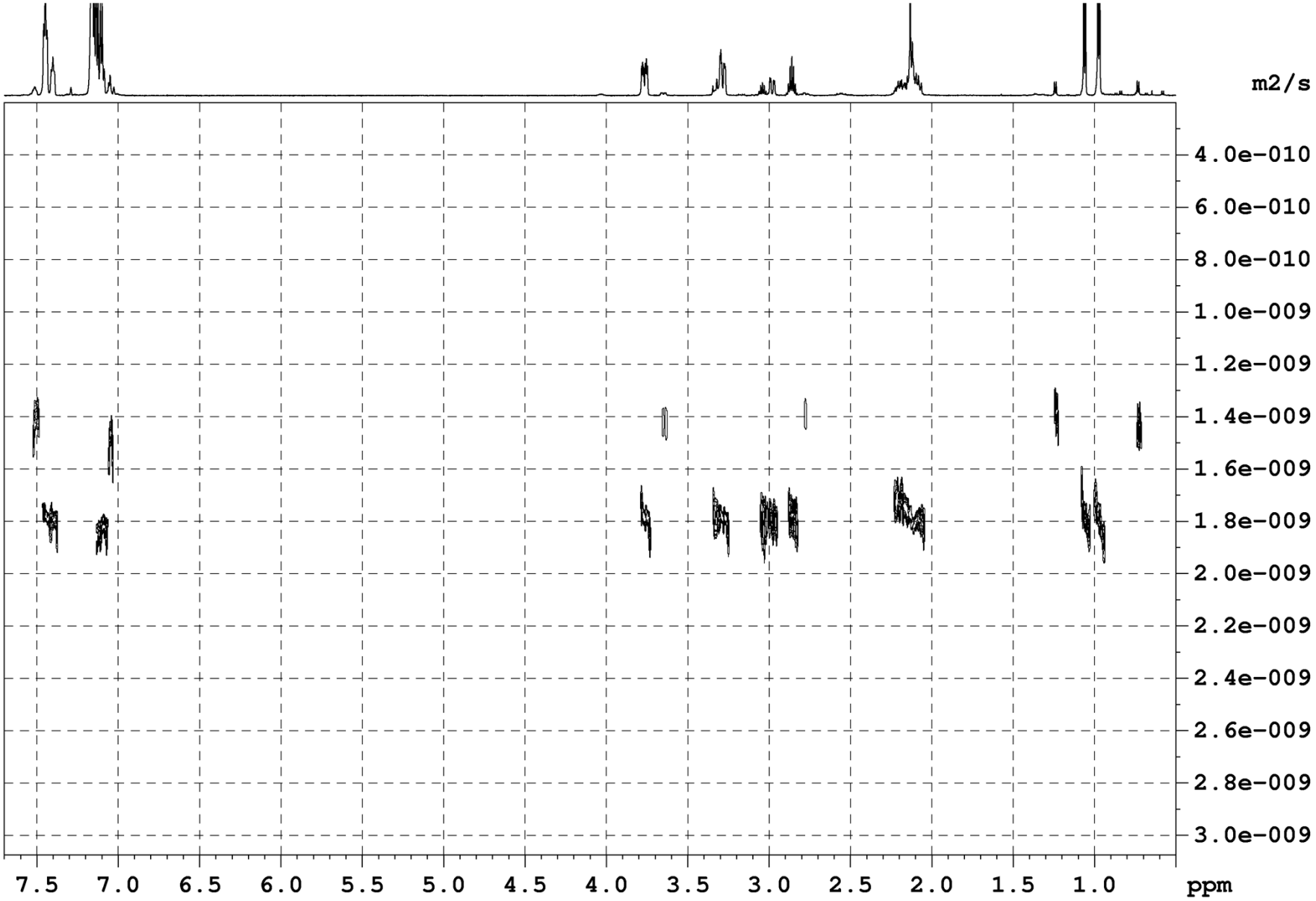


Figure S13. 2D DOSY NMR spectra of **2a**, **2b**, **2c** in C_6D_6 at T = 298 K after ca. 14 days.

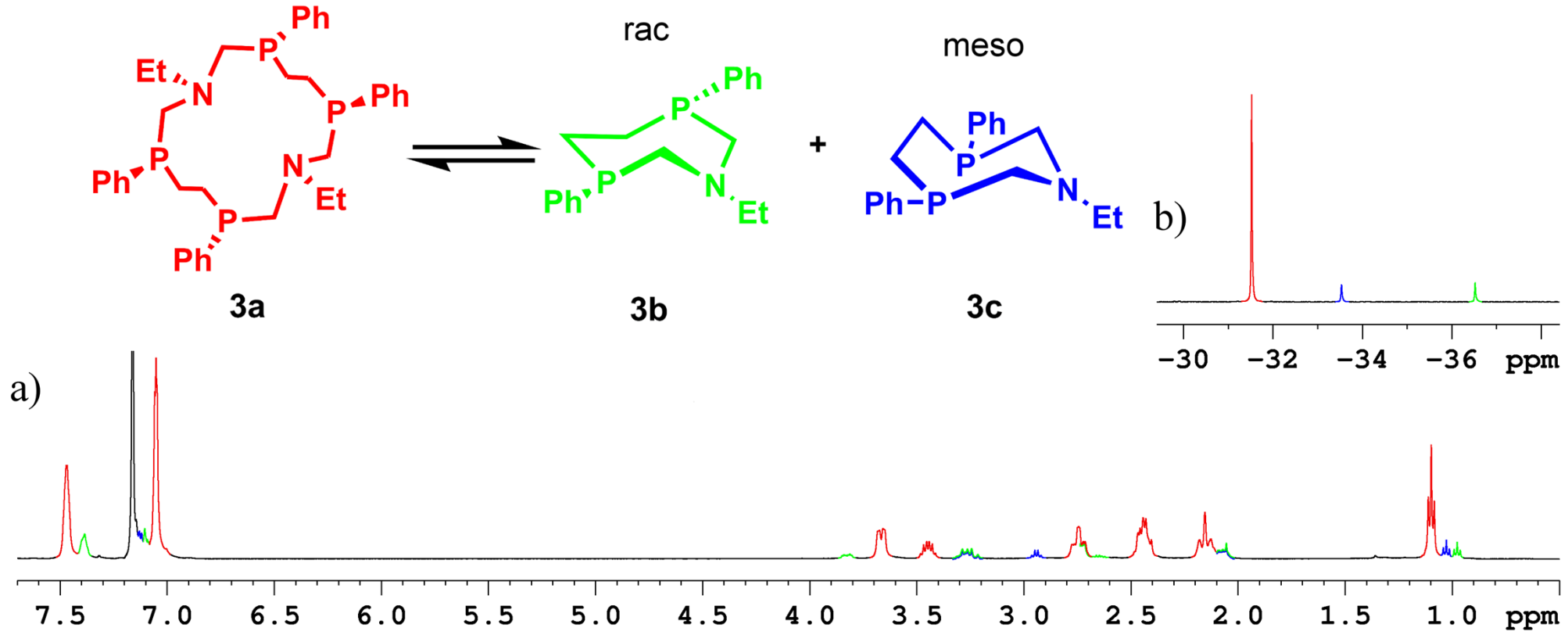


Figure S14. 1D ^{1}H (a) and $^{31}P\{^{1}H\}$ (b) NMR spectra of **3a**, **3b**, **3c** in C_6D_6 at T = 303 K.

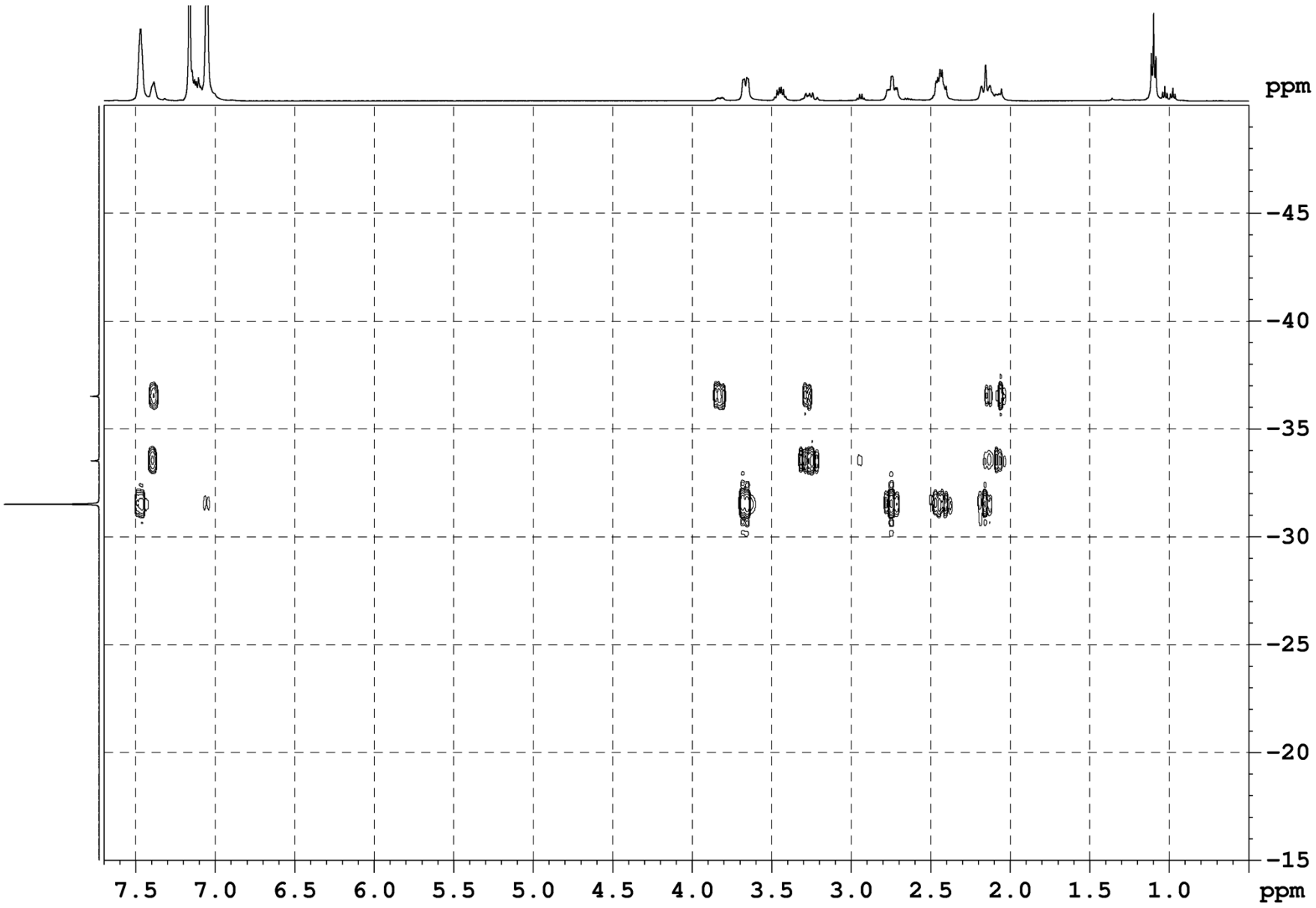


Figure S15. 2D ^{1}H-^{31}P HMBC NMR spectra of **3a**, **3b**, **3c** in C_6D_6 at T = 303 K.

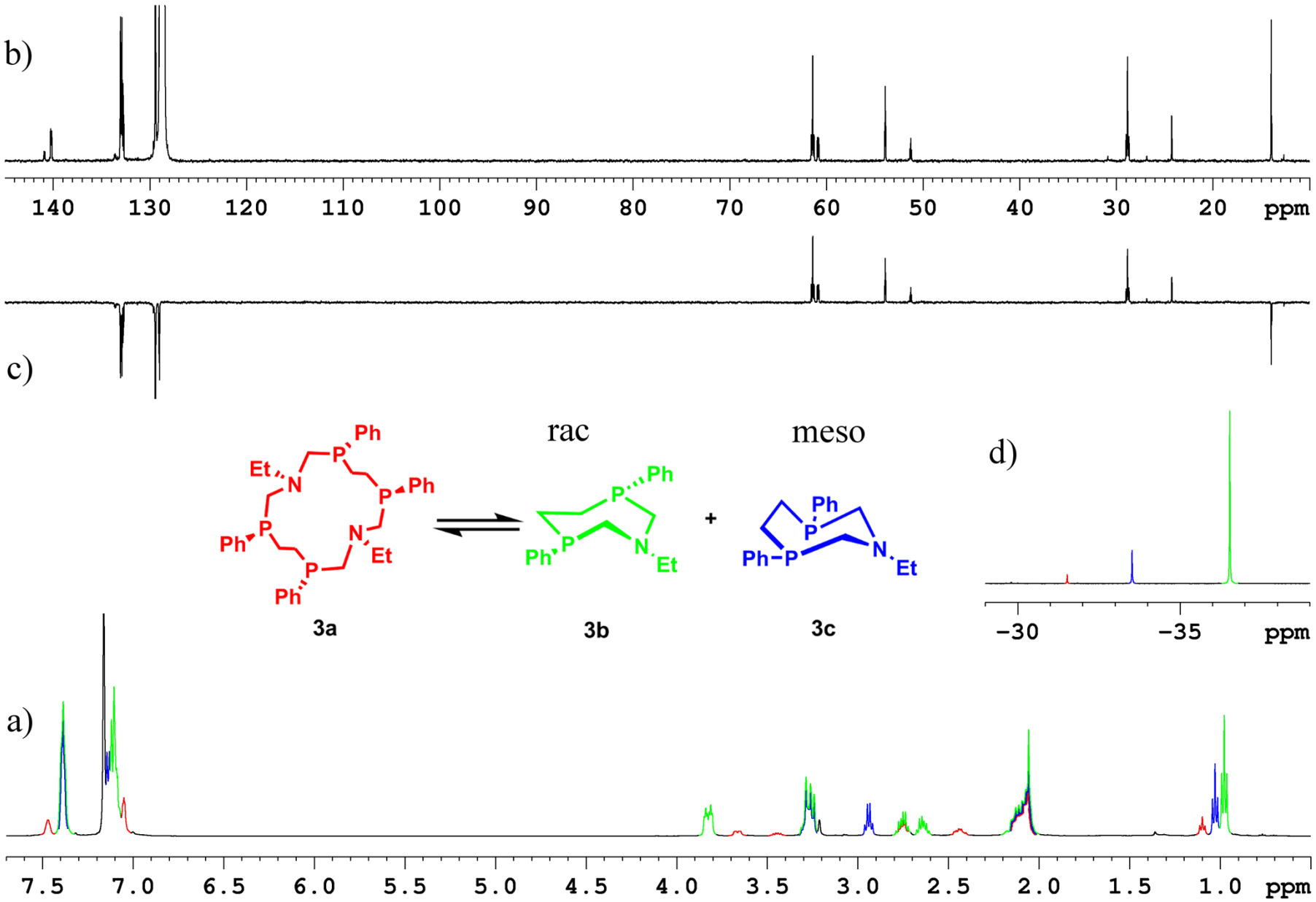


Figure S16. 1D ^{1}H (a), $^{13}C\{^{1}H\}$ (b), ^{13}C DEPT (c), and $^{31}P\{^{1}H\}$(d) NMR spectra of **3a**, **3b**, **3c** in C_6D_6 at T = 303 K after ca. 7 days.

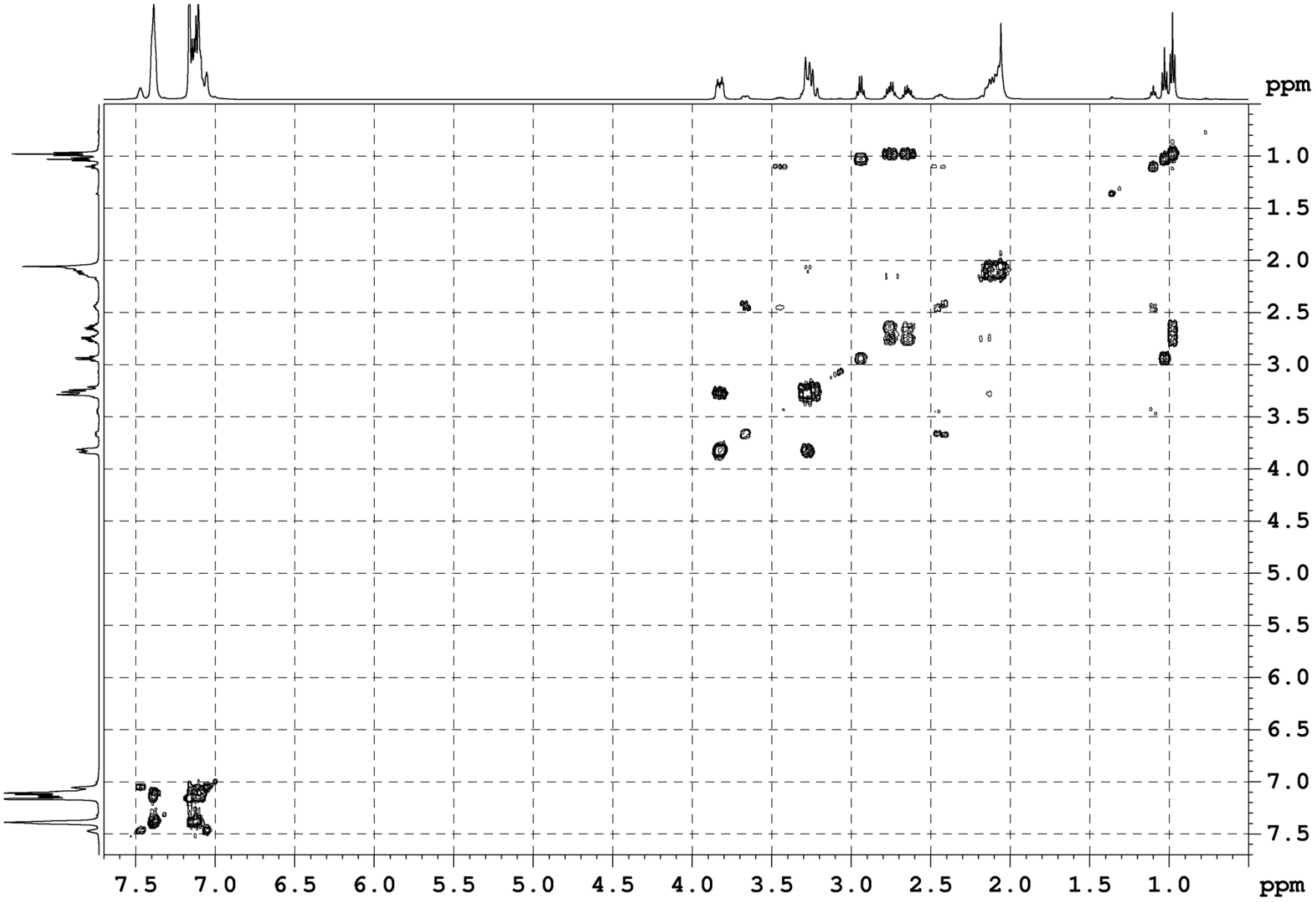


Figure S17. 2D ^{1}H-^{1}H COSY NMR spectra of **3a**, **3b**, **3c** in C_6D_6 at T = 303 K after ca. 7 days.

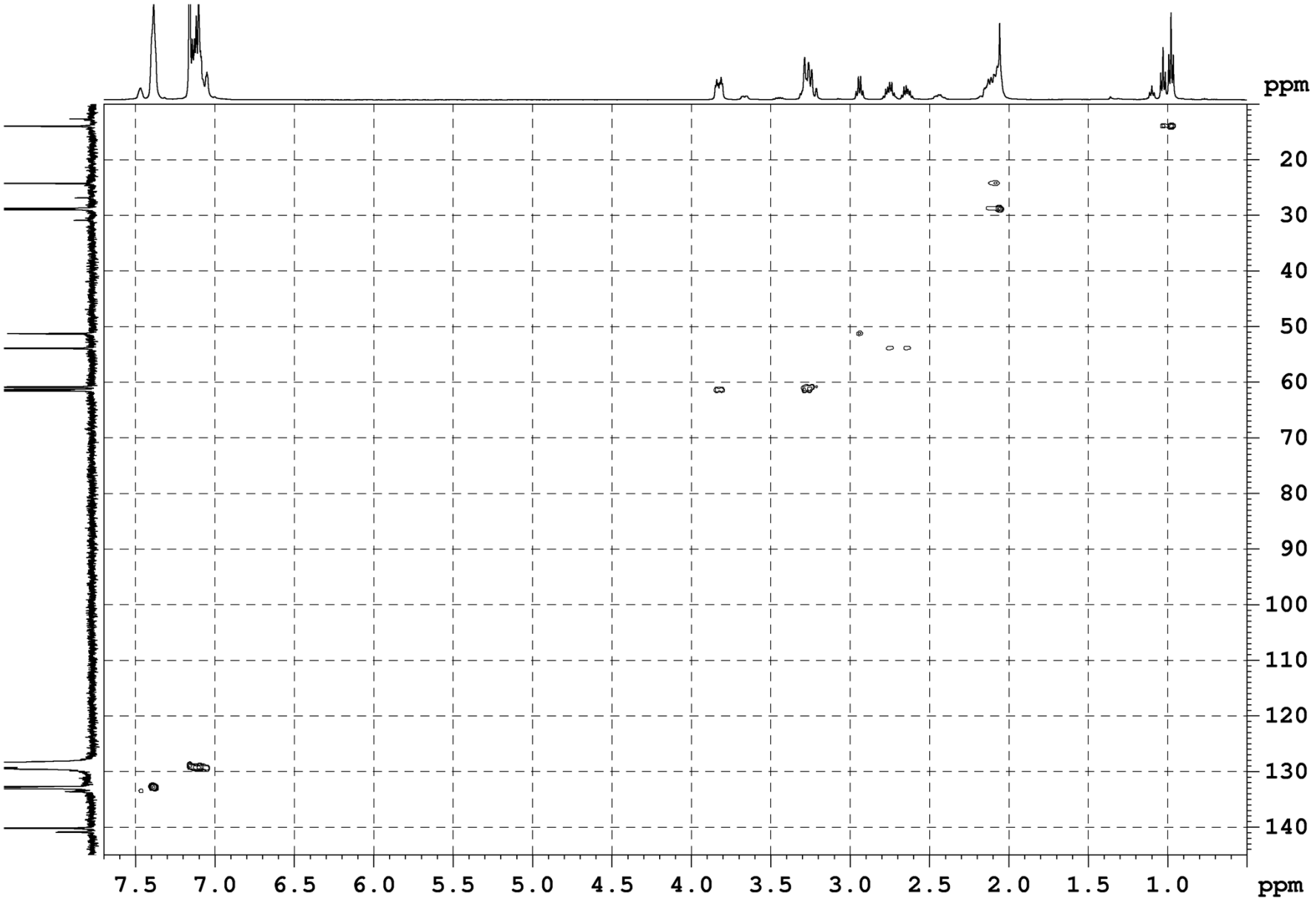


Figure S18. 2D ^{1}H-^{13}C HSQC NMR spectra of **3a**, **3b**, **3c** in C_6D_6 at T = 303 K after ca. 7 days.

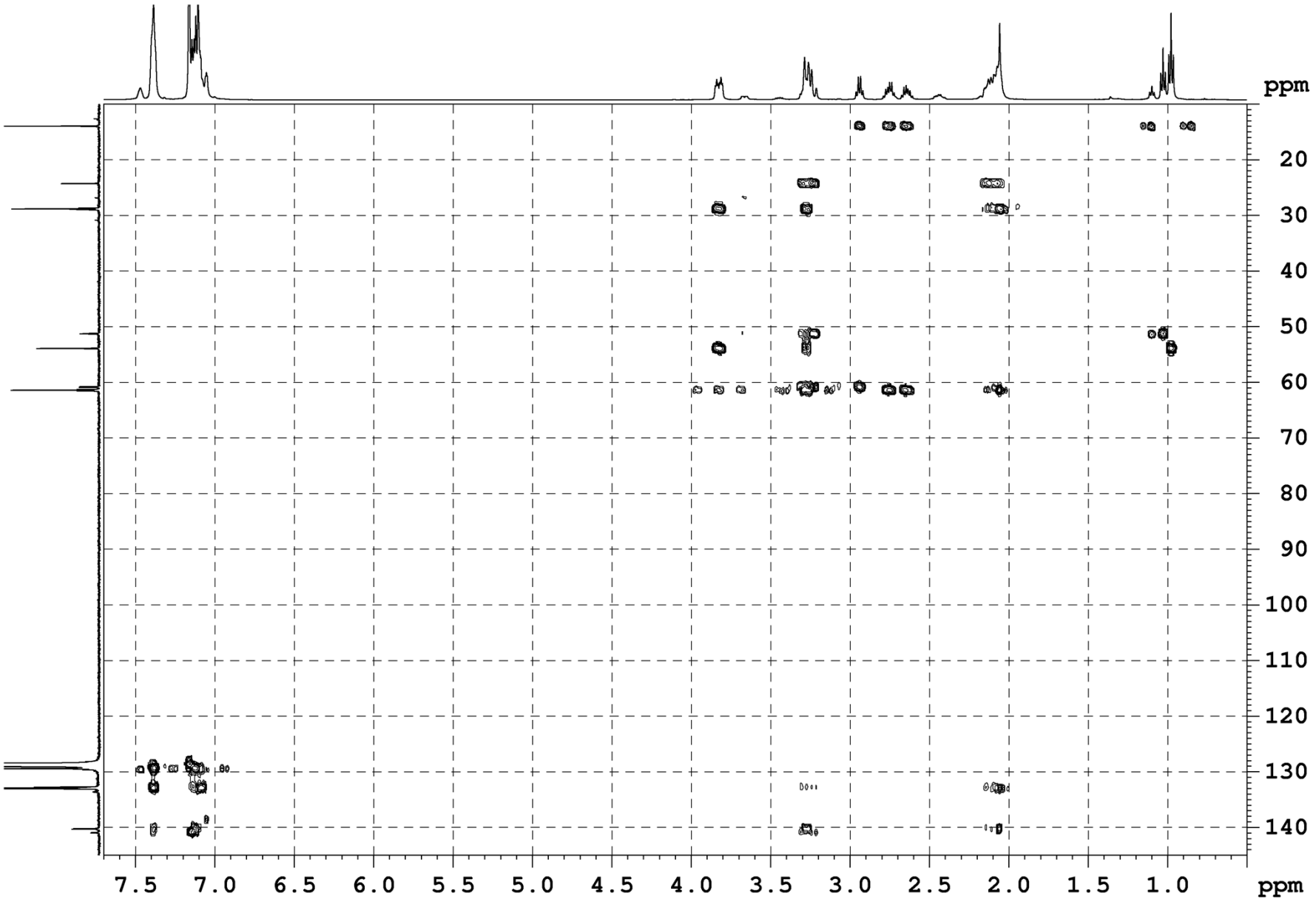


Figure S19. 2D ^{1}H-^{13}C HMBC NMR spectra of **3a**, **3b**, **3c** in C_6D_6 at T = 303 K after ca. 7 days.

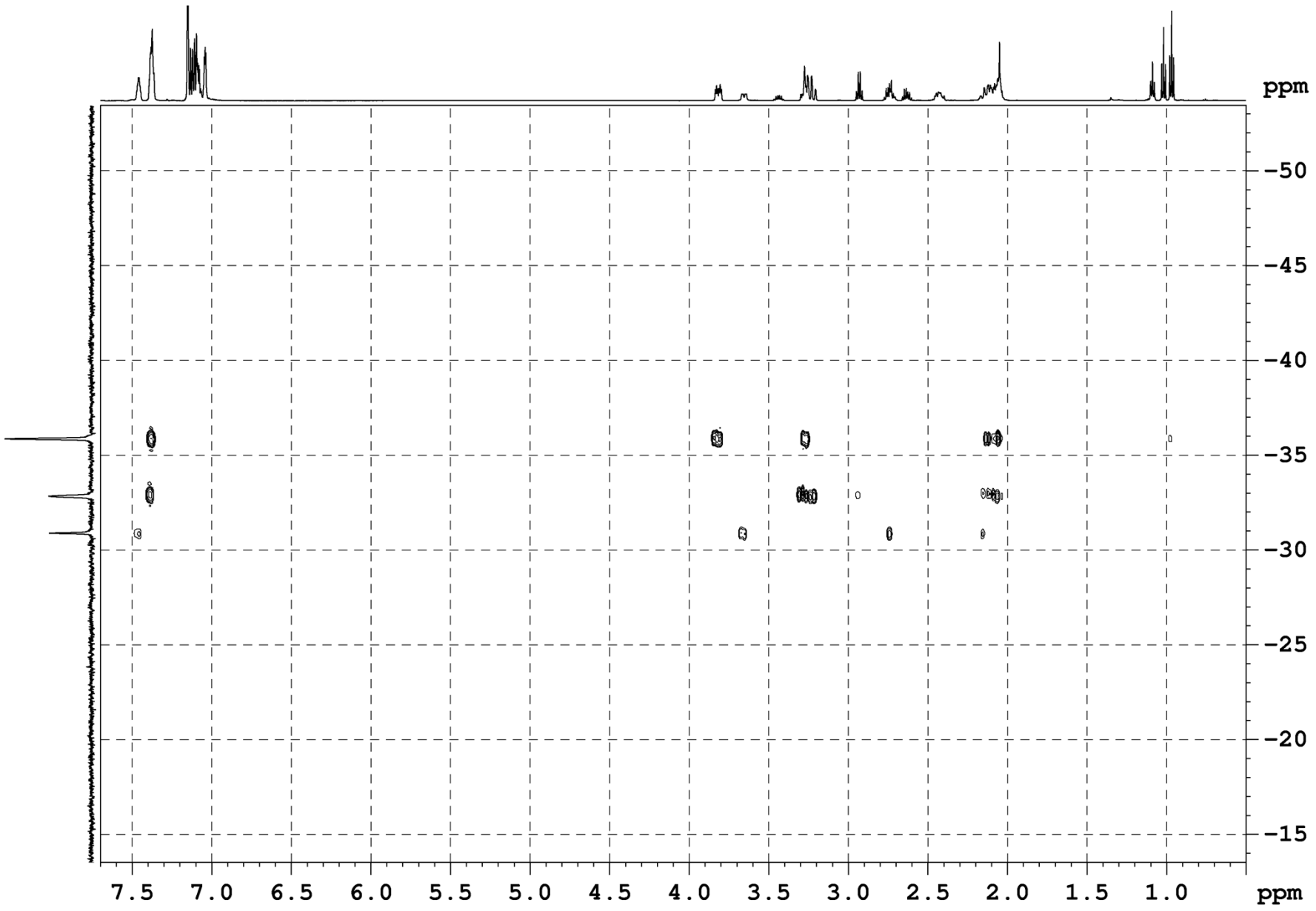


Figure S20. 2D ^{1}H-^{31}P HMBC NMR spectra of **3a**, **3b**, **3c** in C_6D_6 at T = 303 K after ca. 7 days.

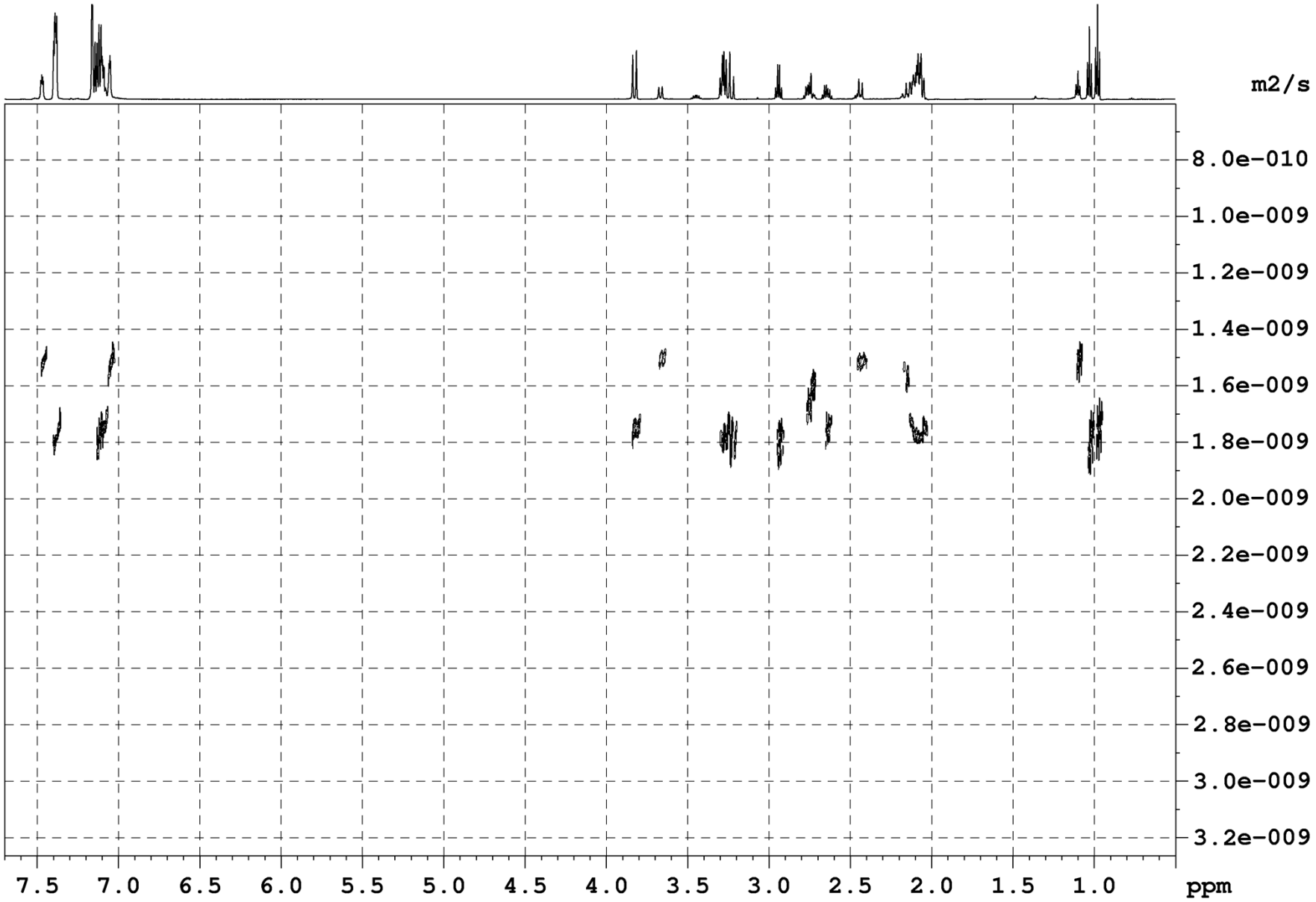


Figure S21. DOSY NMR spectra of **3a**, **3b**, **3c** in C_6D_6 at T = 298 K after ca. 7 days.

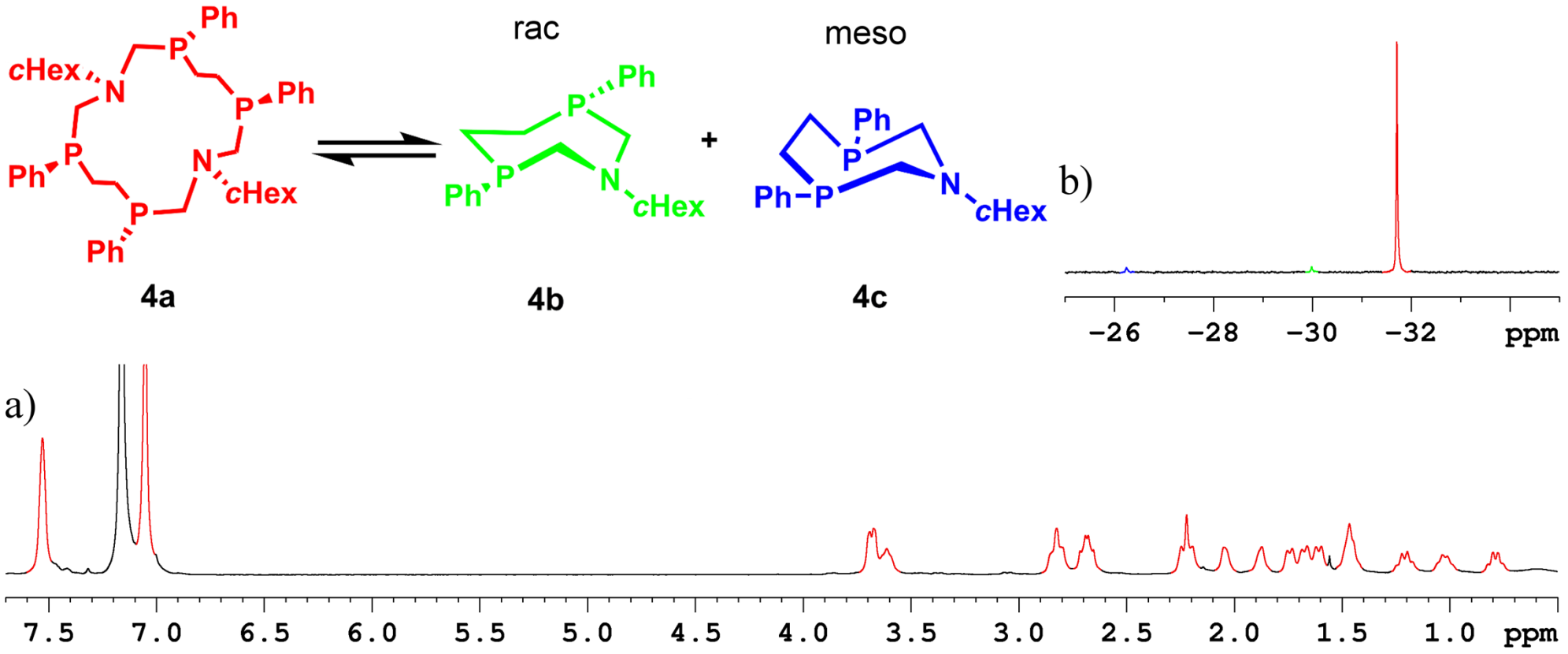


Figure S22. 1D ^{1}H (a) and $^{31}P\{^{1}H\}$ (b) NMR spectra of **4a**, **4b**, **4c** in C_6D_6 at T = 303 K.

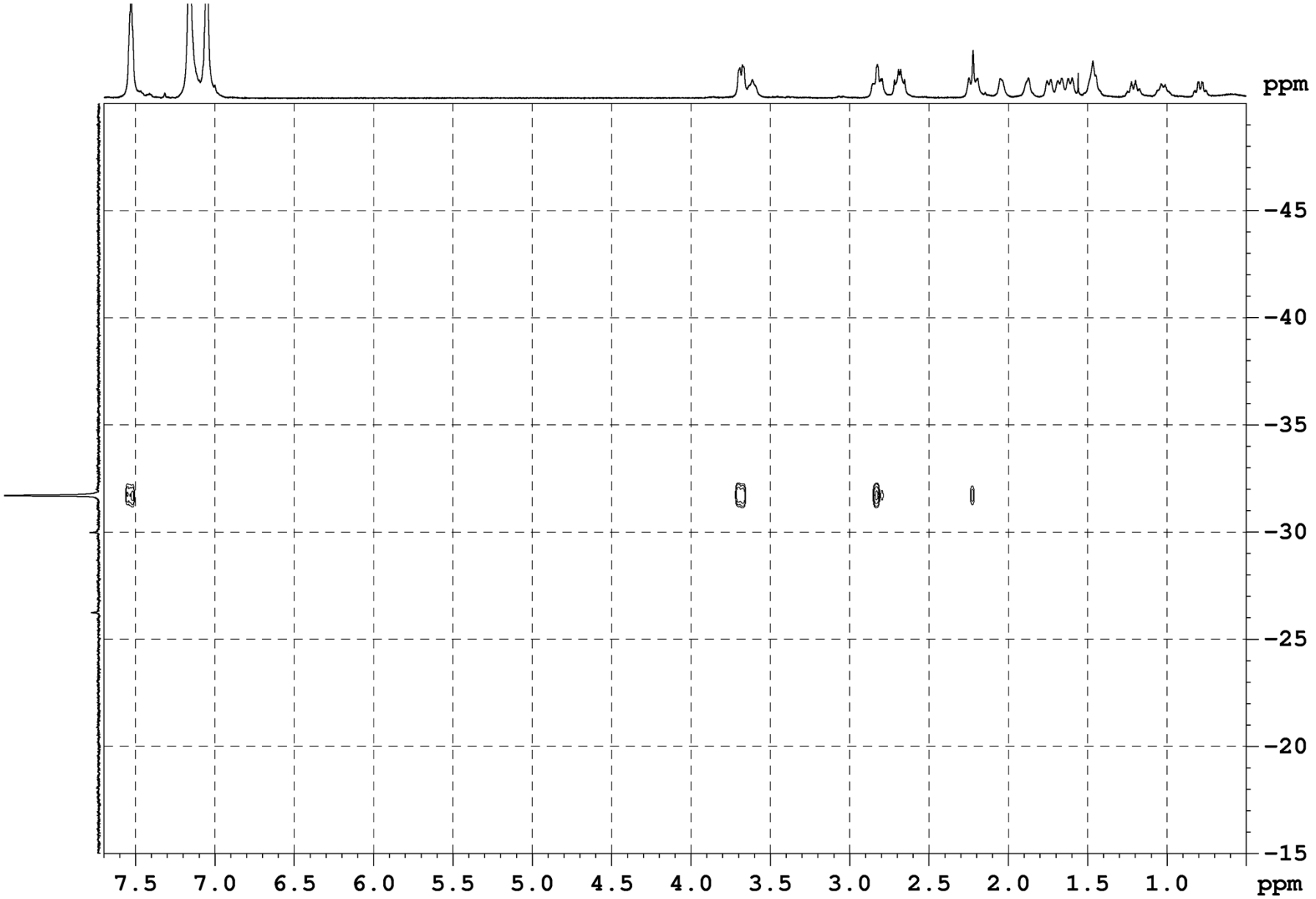


Figure S23. 2D ^{1}H-^{31}P HMBC NMR spectra of **4a**, **4b**, **4c** in C_6D_6 at T = 303 K.

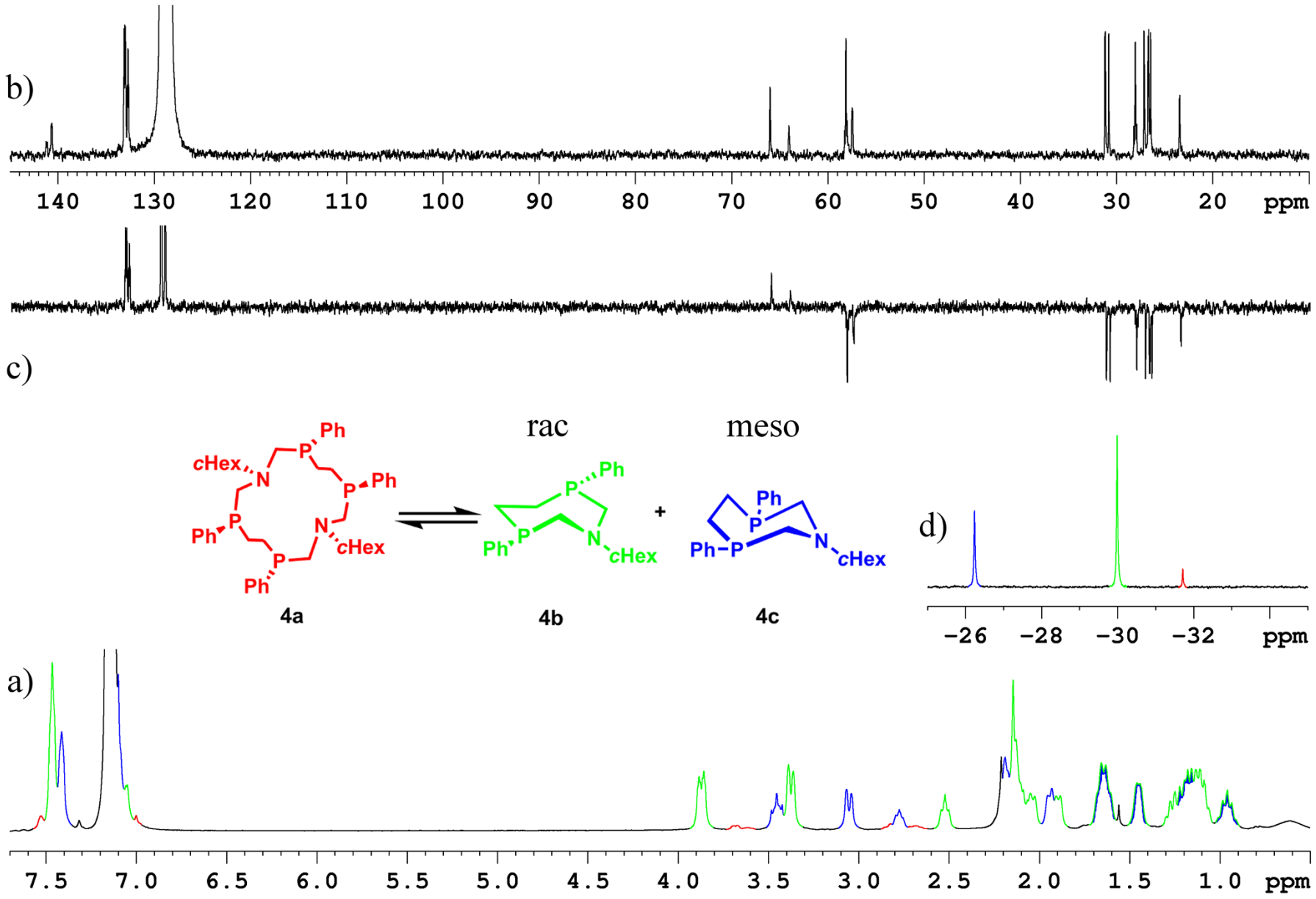


Figure S24. 1D ^{1}H, $^{13}C\{^{1}H\}$, ^{13}C DEPT, and $^{31}P\{^{1}H\}$ NMR spectra of **4a**, **4b**, **4c** in C_6D_6 at T = 303 K after ca. 5 days.

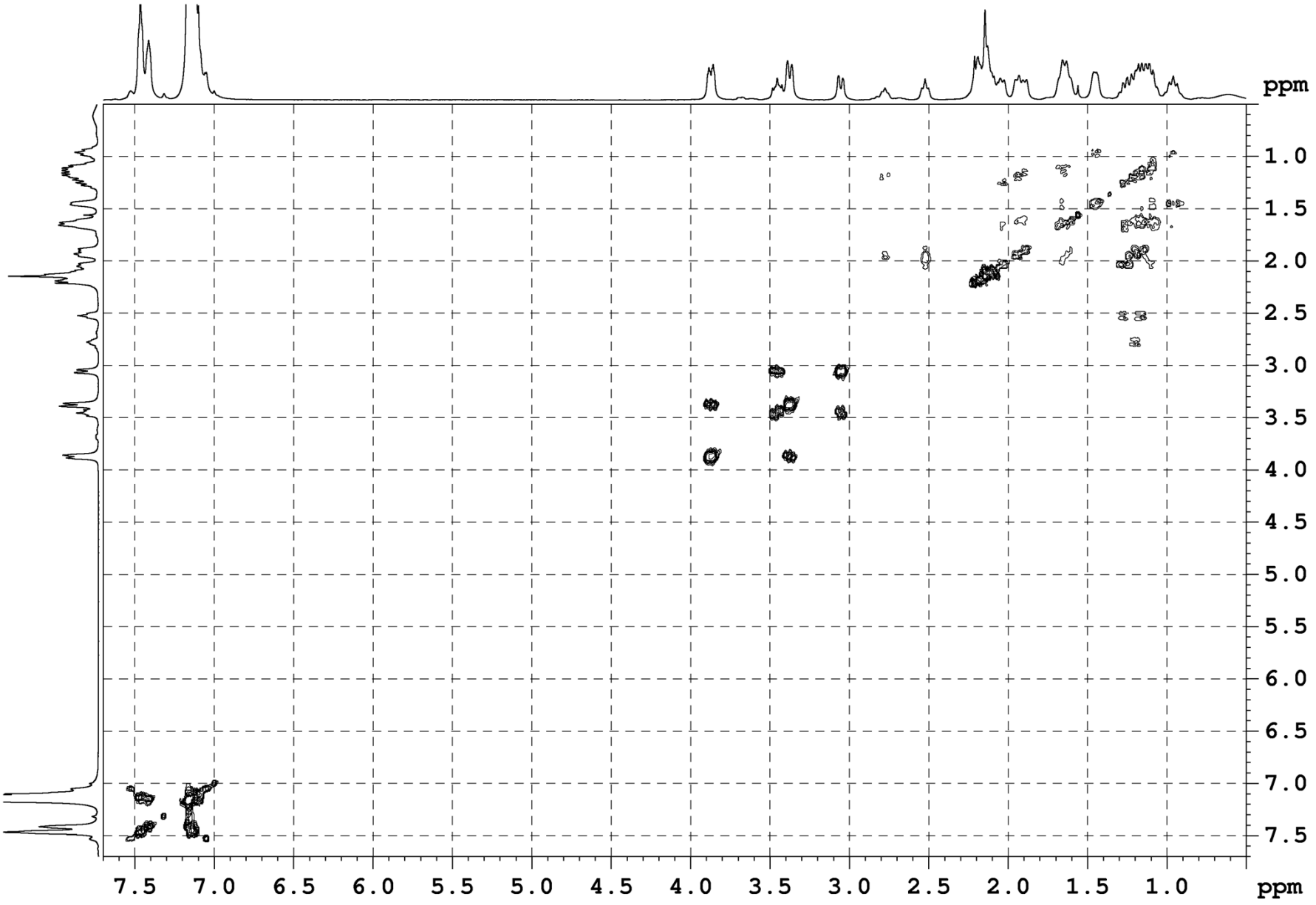


Figure S25. 2D ^{1}H-^{1}H COSY NMR spectra of **4a**, **4b**, **4c** in C_6D_6 at T = 303 K after ca. 5 days.

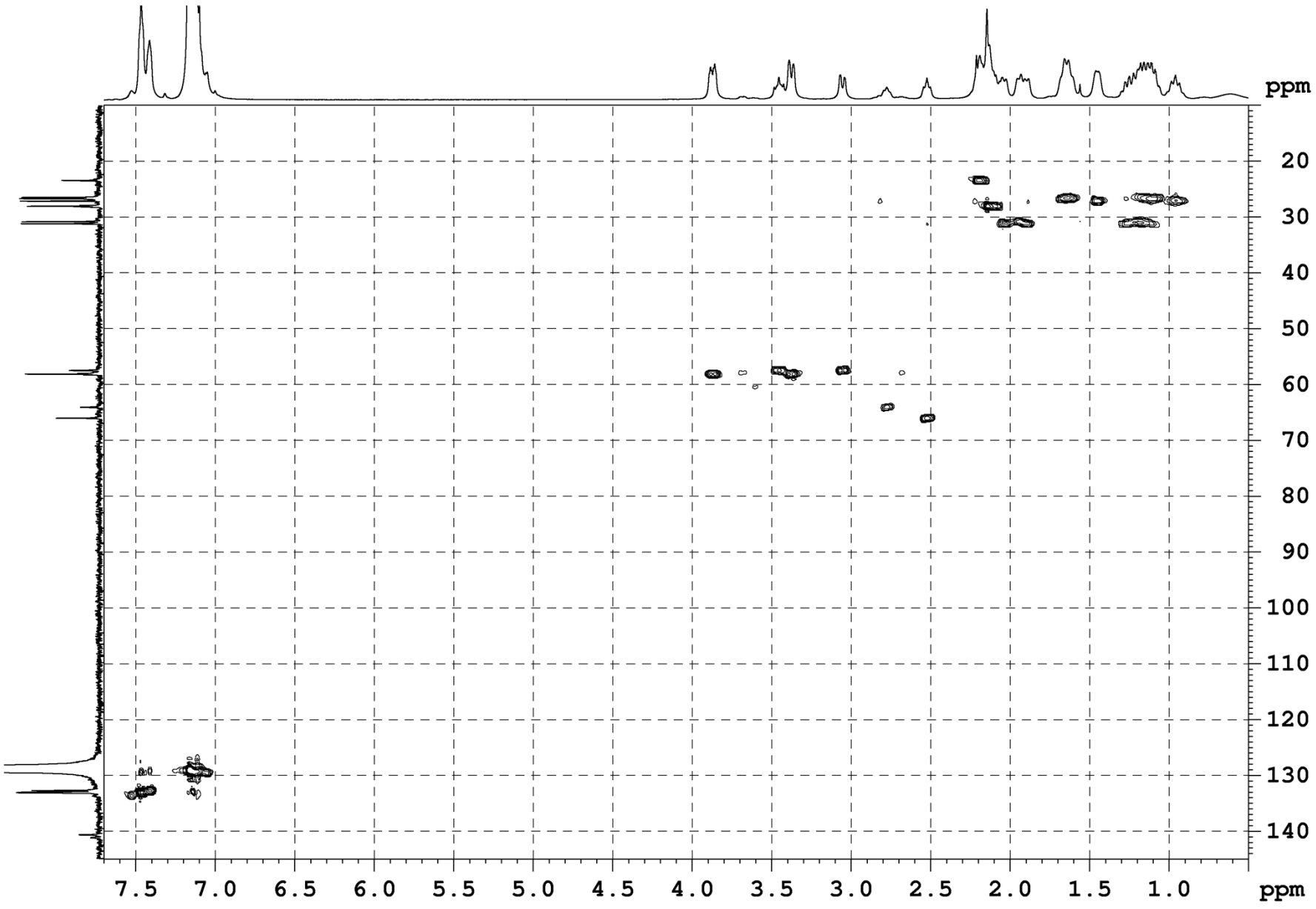


Figure S26. 2D ^{1}H-^{13}C HSQC NMR spectra of **4a**, **4b**, **4c** in C_6D_6 at T = 303 K after ca. 5 days.

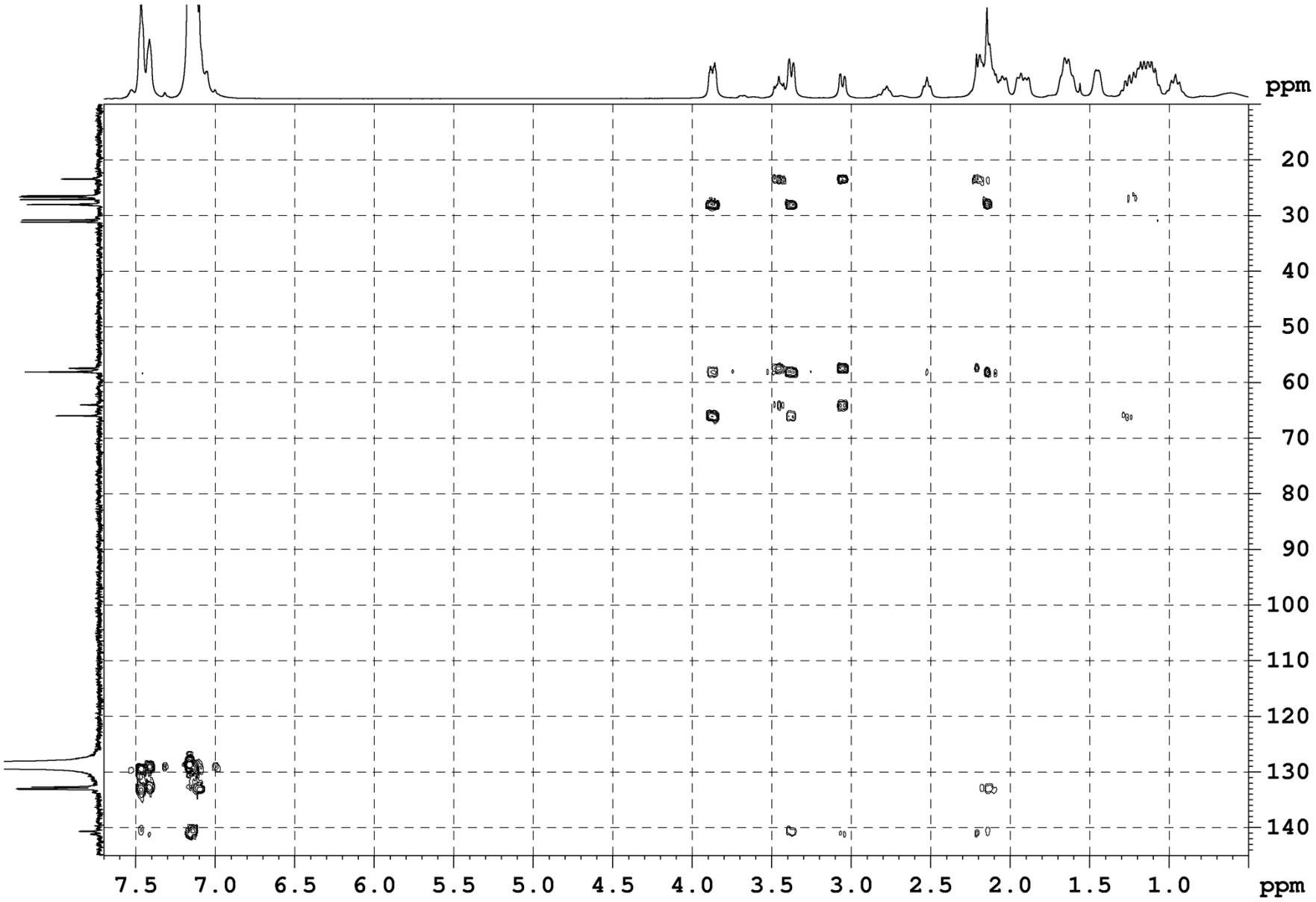


Figure S27. 2D ^{1}H-^{13}C HMBC NMR spectra of **4a**, **4b**, **4c** in C_6D_6 at T = 303 K after ca. 5 days.

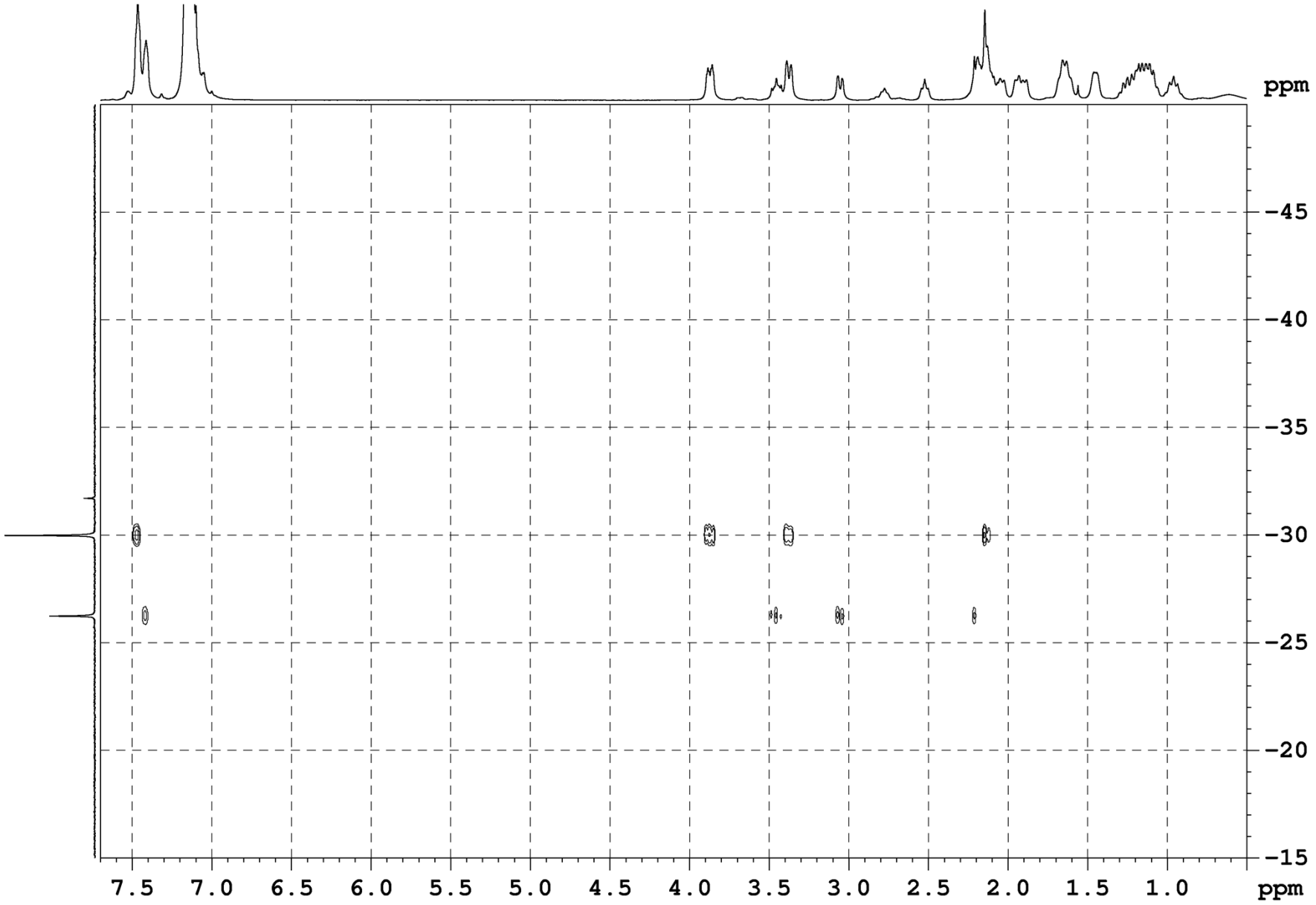


Figure S28. 2D ^{1}H-^{31}P HMBC NMR spectra of **4a**, **4b**, **4c** in C_6D_6 at T = 303 K after ca. 5 days.

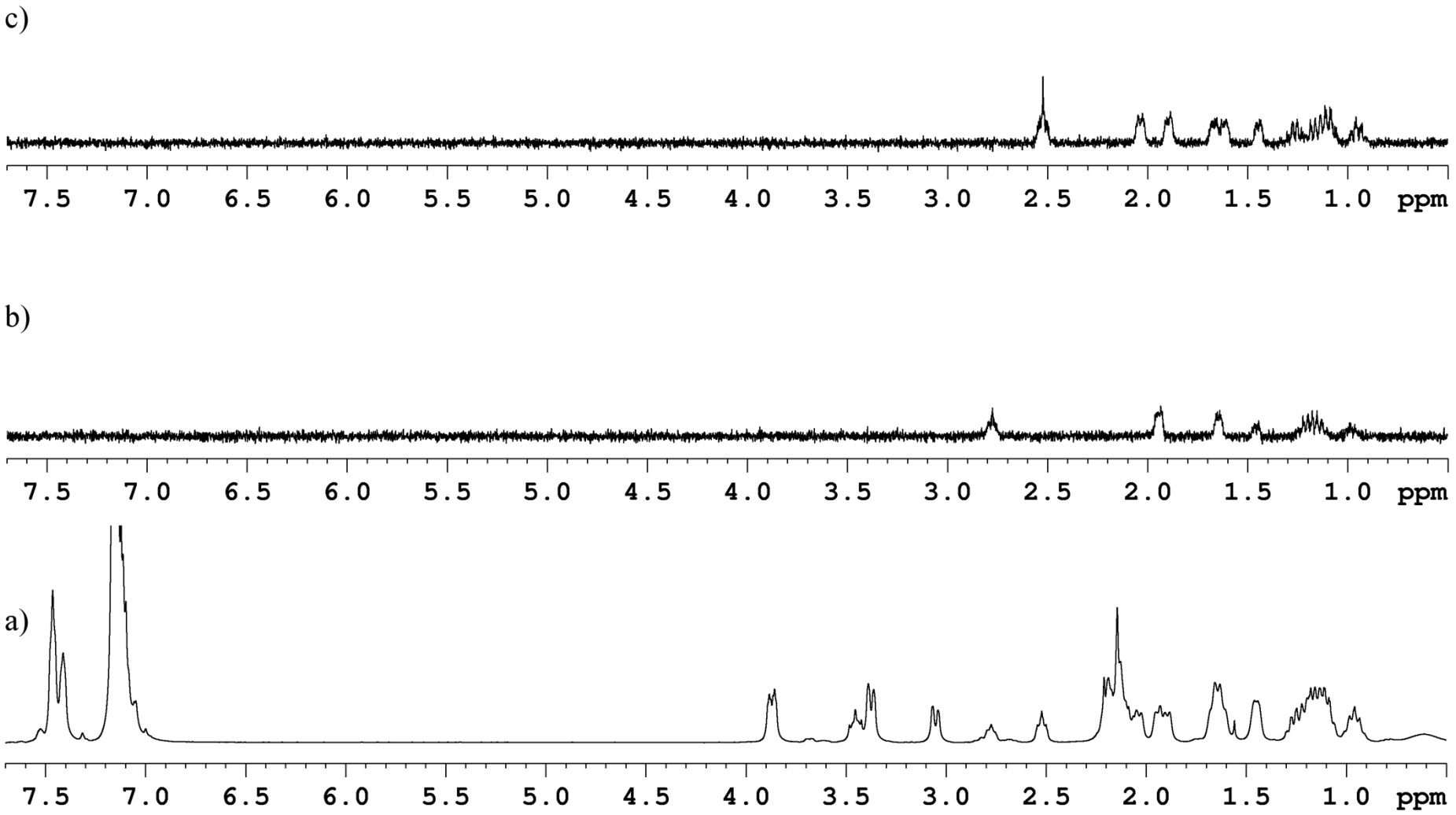
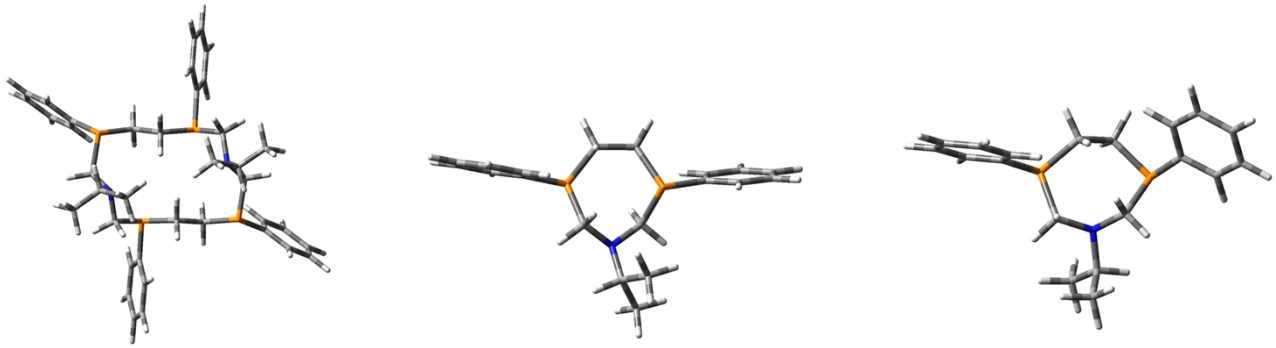


Figure S29. 1D ^{1}H (a) and 1D TOCSY (b, c) NMR spectra of **4a**, **4b**, **4c** in C_6D_6 at T = 303 K after ca. 5 days.

Calculations

The quantum chemical calculations were performed using Gaussian 03w software package. Full geometry optimizations have been carried out within the framework of DFT (PBE1PBE) method using 6-31+G(d) basis sets. Chemical shifts (CSs) were calculated by the GIAO method at the PBE1PBE/6-311G(2d,2p) level of theory. ^{31}P CSs were referred at H_3PO_4. Linear scaling procedure was applied for correcting systematic errors ($\delta_{scaled} = (\delta_{unscaled} - intercept)/slope$, where intepcept = -14.4 ppm, slope = 1.073).[1]



2a
E = -2950.6215279 Hartree

2b
E = -1475.3026782 Hartree

2c
E = -1475.3002833 Hartree

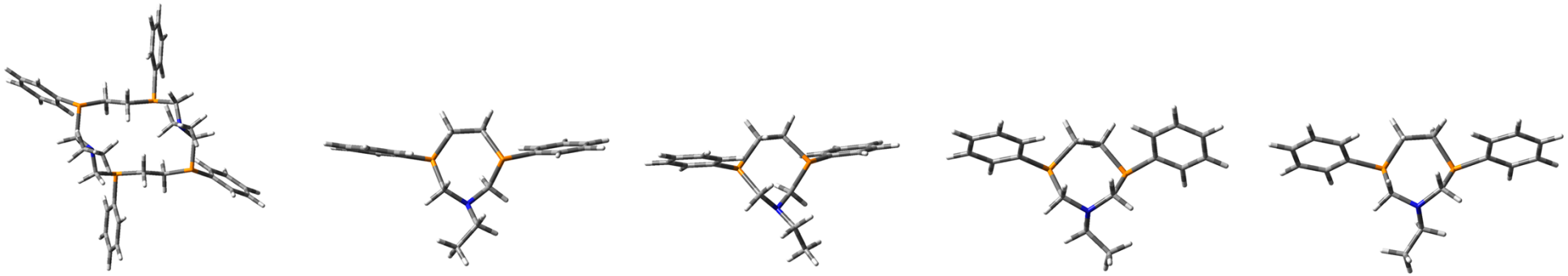
Figure S30. Optimized structures of **2a**, **2b** and **2c** at the PBE1PBE/6-31+G(d) level of theory.

Table S1. Calculated ^{31}P CS's[a] for **2a**, **2b**, **2c**.

Compounds	Unscaled			Scaled
	δ_{P1}	δ_{P2}	δ_{av}[b]	δ_{scaled}[b]
2a	-49.2	-53.1	-51.2	-33.5
2b	-47.3	-52.5	-49.9	-32.3
2c	-33.7	-45.2	-39.5	-22.8

[a] CS's calculated at PBE1PBE/6-311G(2d,2p) with geometry optimized at PBE1PBE/6-31+G(d) level of theory; [b] CS's averaged between δ_{P1} and δ_{P2}, $\delta_{av} = (\delta_{P1} + \delta_{P2})/2$.

[1] Sh. K. Latypov, F. M. Polyancev, D. G. Yakhvarov and O. G. Sinyashin, *Phys. Chem. Chem. Phys.*, 2015, **17**, 6976—6987.



3a
E = -2872.0910879 Hartree

3b+g
E = -1436.0384999 Hartree

3b-g
E = -1436.0383751 Hartree

3c+g
E = -1436.0364011 Hartree

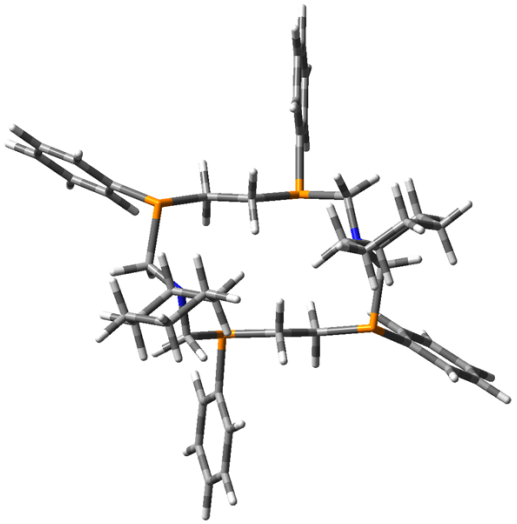
3c-g
E = -1436.0365397 Hartree

Figure S31. Optimized structures of **3a**, **3b+g**, **3b-g**, **3c+g**, **3c-g** at the PBE1PBE/6-31+G(d) level of theory.

Table S2. Calculated ^{31}P CS's[a] for **3a**, **3b+g**, **3b-g**, **3c+g**, **3c-g**.

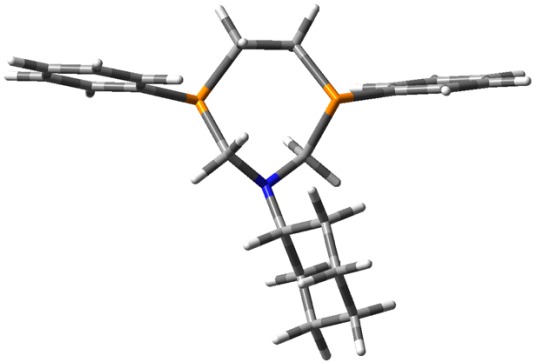
Compounds	Unscaled			Scaled
	δ_{P1}	δ_{P2}	δ_{av}[b]	δ_{scaled}[b]
3a	-49.5	-53.4	-51.5	-33.7
3b+g	-54.8	-70.3	-62.6	-43.8
3b-g	-50.4	-74.2	-62.3	-43.5
3c+g	-44.8	-49.7	-47.3	-29.9
3c-g	-54.8	-70.3	-62.6	-43.8

[a] CS's calculated at PBE1PBE/6-311G(2d,2p) with geometry optimized at PBE1PBE/6-31+G(d) level of theory; [b] CS's averaged between δ_{P1} and δ_{P2}, $\delta_{av} = (\delta_{P1} + \delta_{P2})/2$.



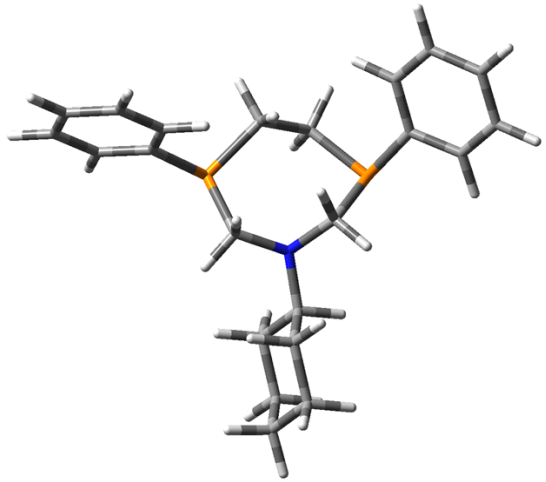
4a

E = -3183.8308828 Hartree



4b

E = -1591.9074875 Hartree



4c

E = -1591.9051614 Hartree

Figure S32. Optimized structures of **4a**, **4b**, **4c** at the PBE1PBE/6-31+G(d) level of theory.

Table S3. Calculated ^{31}P CS[a] for **4a**, **4b**, **4c**.

Compounds	Unscaled			Scaled
	δ_{P1}	δ_{P2}	δ_{av}[b]	δ_{scaled}[b]
4a	-49.4	-52.6	-51.0	-33.3
4b	-46.7	-52.8	-49.4	-32.3
4c	-33.9	-45.6	-39.8	-23.1

[a] CS's calculated at PBE1PBE/6-311G(2d,2p) with geometry optimized at PBE1PBE/6-31+G(d) level of theory; [b] CS's averaged between δ_{P1} and δ_{P2}, $\delta_{av} = (\delta_{P1} + \delta_{P2})/2$.

Kinetics of dissociation of 2a.

Table S4 Dependence of concentrations of compounds **2a-c** on standing time at 295.5 K; initial concentration of **2a** is 40 mmol/l .

	Concentration, mmol/l		
time, h	c_a	c_b	c_c
0.20	30.77	4.31	4.92
20	15.50	13.02	11.47
93	3.10	23.44	13.46
121.5	2.07	25.13	12.79
140.5	1.65	26.05	12.30
169	1.55	27.20	11.25
188	1.47	27.95	10.58
261	1.47	28.66	9.87
290	1.41	28.70	9.99
309	1.40	28.79	9.78
357	1.35	29.45	9.20
483	1.33	29.49	9.08
500	1.32	29.63	8.95
550	1.26	29.79	8.94
649	1.23	29.76	8.96

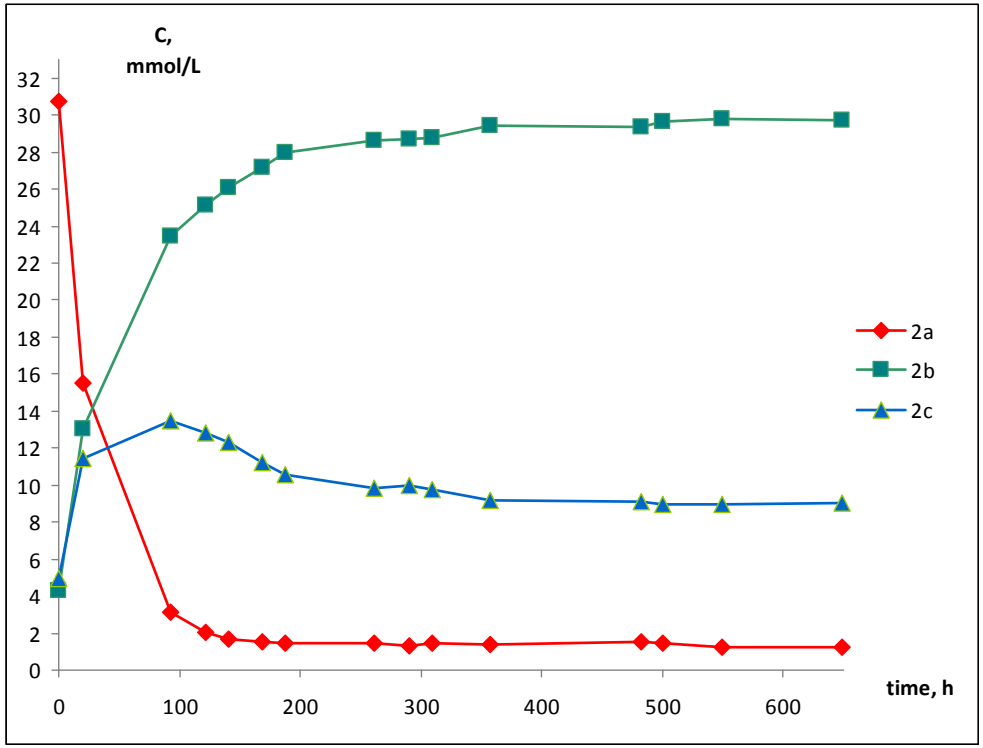


Table S5. Dependence of concentrations of compounds**2a-c** on standing time at 295.5 K;initial concentration of **2a** is 10 mmol/l.

	Concentration, mmol/l		
time, h	c_a	c_b	c_c
0	10	0	0
20.5	10	0	0
73	7.35	1.32	1.32
101.5	7.04	1.41	1.55
119.5	6.41	1.67	1.92
167.5	5.21	2.71	2.08
240	3.31	3.97	2.71
287	2.26	4.39	3.35
336	1.30	5.02	3.69
462	0.75	5.81	3.55
479	0.72	5.76	3.52
528.5	0.43	5.98	3.48
627	0.25	6.49	3.26
648	0.18	6.67	3.14

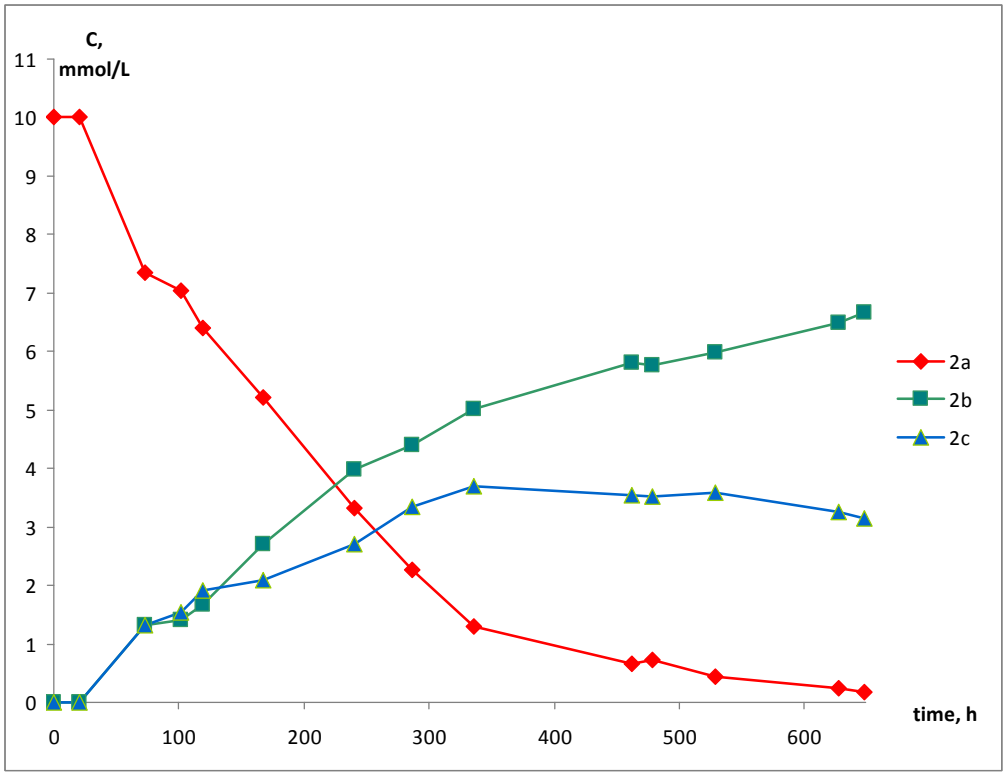


Table S6. Dependenceof concentrations of compounds **2a-c** on standing time at 343 K; initial concentration of **2a** is 10 mmol/l .

	Concentration, mmol/l		
time, h	c_a	c_b	c_c
0	10	0	0
2.5	6.76	1.76	1.48
4	5.05	2.63	2.32
5.3	4.03	3.31	2.66
6.2	3.62	3.41	2.97
7.1	3.31	3.58	3.11
8.1	2.75	3.85	3.41
9.1	2.49	4.23	3.28
23.6	0.35	6.12	3.53
29.5	0.13	6.31	3.55
31	0.13	6.55	3.32
48	0.02	6.93	3.05

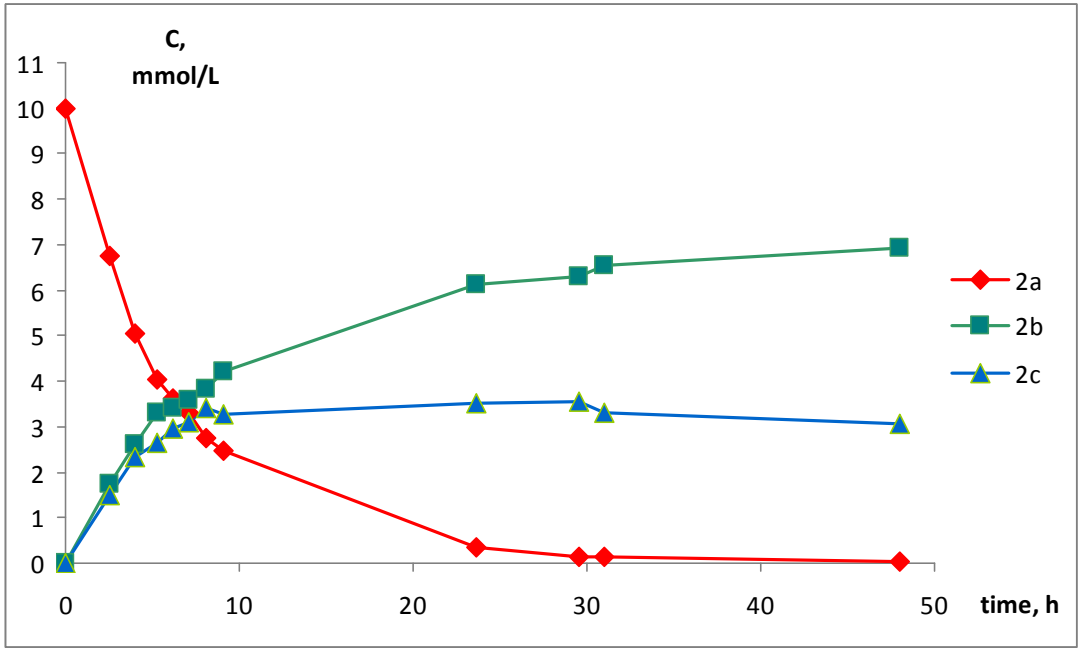
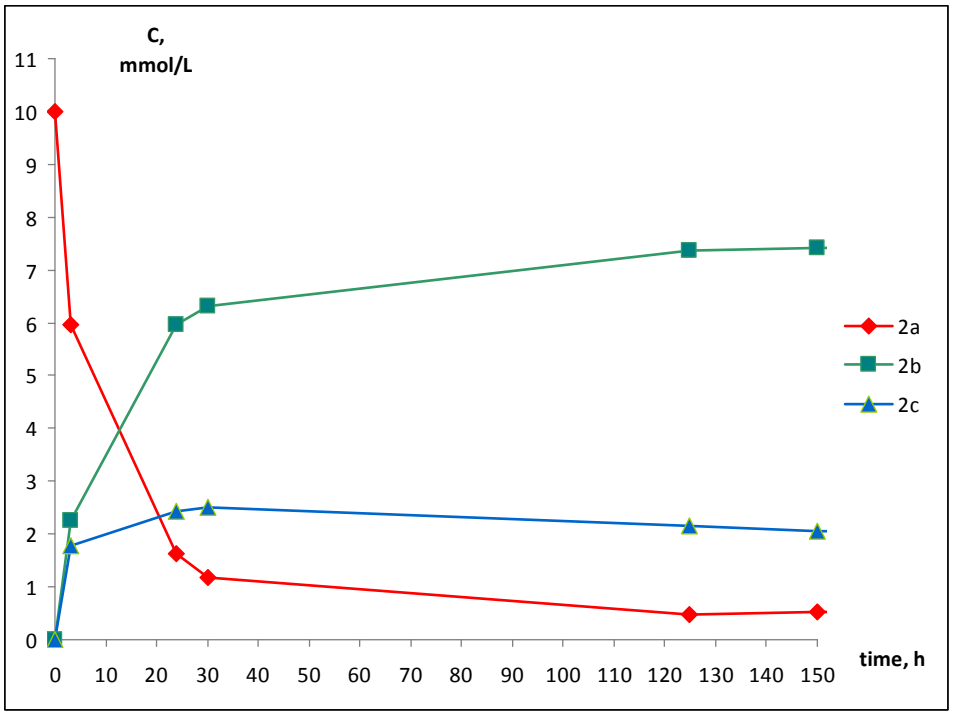


Table S7. Dependenceof concentrations of compounds **2a-c** on standing time at 293 K;

initial concentration of **2a** is 10 mmol/l in the presence of 10% of p-toluolsulfonic acid.

	Concentration, mmol/l		
time, h	c_a	c_b	c_c
0	10	0	0
3	5.95	2.26	1.78
24	1.62	5.95	2.43
30	1.18	6.32	2.50
124.8	0.48	7.36	2.15
149.9	0.51	7.43	2.06
293.9	0.46	7.49	2.04
364	0.57	7.26	2.17
483.2	0.52	7.30	2.17



X-Ray Crystallography.

Table S8. Crystal data and structure refinement for **2a**.

Identification code	x0894fin	
Empirical formula	C38 H50 N2 P4	
Formula weight	658.68	
Temperature	130(2) K	
Wavelength	71.073 pm	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 2124.85(4) pm	□= 90°.
	b = 813.730(10) pm	□= 106.726(2)°.
	c = 2178.57(4) pm	□ = 90°.
Volume	3.60750(11) nm^3	
Z	4	
Density (calculated)	1.213 Mg/m^3	
Absorption coefficient	0.238 mm^{-1}	
F(000)	1408	
Crystal size	0.5 x 0.4 x 0.3 mm^3	
Theta range for data collection	2.964 to 30.503°.	
Index ranges	-30<=h<=28, -11<=k<=11, -31<=l<=31	
Reflections collected	17896	
Independent reflections	5502 [R(int) = 0.0208]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1 and 0.99257	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5502 / 45 / 299	

Goodness-of-fit on F^2	1.053
Final R indices [I>2sigma(I)]	R1 = 0.0322, wR2 = 0.0893
R indices (all data)	R1 = 0.0438, wR2 = 0.0923
Extinction coefficient	n/a
Largest diff. peak and hole	0.447 and -0.217 e.$Å^{-3}$

Comments: Structure solution with SIR92 (Direct method). Anisotropic refinement of all non-hydrogen atoms with SHELXL-2014. All H atoms were located on difference Fourier maps calculated at the final stage of the structure refinement. Restraints are only used to model hydrogen atoms of the methyl substituents C(6) and C(7).

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	4011(1)	1134(1)	3023(1)	19(1)
P(2)	3725(1)	346(1)	926(1)	19(1)
N(1)	5005(1)	-960(1)	3673(1)	18(1)
C(1)	5401(1)	311(2)	4082(1)	22(1)
C(2)	4304(1)	-638(1)	3571(1)	21(1)
C(3)	4001(1)	183(1)	2254(1)	21(1)
C(4)	3800(1)	1397(2)	1692(1)	23(1)
C(5)	5205(1)	-2638(2)	3914(1)	30(1)
C(6)	4921(1)	-3893(2)	3398(1)	71(1)
C(7)	5056(1)	-3054(3)	4543(1)	67(1)
C(8)	3149(1)	1035(1)	3022(1)	18(1)
C(9)	2642(1)	279(2)	2551(1)	25(1)
C(10)	2004(1)	260(2)	2596(1)	30(1)
C(11)	1858(1)	985(2)	3113(1)	30(1)
C(12)	2356(1)	1732(2)	3588(1)	29(1)
C(13)	2990(1)	1766(2)	3538(1)	23(1)
C(14)	3464(1)	1972(1)	326(1)	19(1)
C(15)	3228(1)	1443(2)	-307(1)	24(1)
C(16)	3040(1)	2559(2)	-809(1)	27(1)
C(17)	3074(1)	4216(2)	-683(1)	28(1)
C(18)	3298(1)	4774(2)	-55(1)	30(1)
C(19)	3496(1)	3658(2)	445(1)	27(1)

Table S10. Bond lengths [pm] and angles [°] for x0894fin.

P(1)-C(8)	183.48(11)
P(1)-C(3)	183.87(11)
P(1)-C(2)	186.20(11)
P(2)-C(14)	182.89(11)
P(2)-C(4)	184.11(12)
P(2)-C(1)#1	186.28(11)
N(1)-C(1)	146.33(14)
N(1)-C(2)	146.54(13)
N(1)-C(5)	148.12(15)
C(1)-P(2)#1	186.27(11)
C(1)-H(1A)	98.8(16)
C(1)-H(1B)	98.9(14)
C(2)-H(2A)	100.2(14)
C(2)-H(2B)	103.0(14)
C(3)-C(4)	153.49(15)
C(3)-H(3A)	96.0(13)
C(3)-H(3B)	103.1(15)
C(4)-H(4A)	102.2(15)
C(4)-H(4B)	98.1(14)
C(5)-C(6)	151.1(2)
C(5)-C(7)	153.0(2)
C(5)-H(5)	96.8(13)
C(6)-H(6A)	94.8(10)
C(6)-H(6B)	94.2(10)
C(6)-H(6C)	93.0(10)

C(7)-H(7A)	94.1(10)
C(7)-H(7B)	94.5(10)
C(7)-H(7C)	92.4(10)
C(8)-C(13)	139.65(15)
C(8)-C(9)	139.78(15)
C(9)-C(10)	138.75(17)
C(9)-H(9)	92.9(15)
C(10)-C(11)	138.34(19)
C(10)-H(10)	97.0(16)
C(11)-C(12)	138.82(19)
C(11)-H(11)	90.8(14)
C(12)-C(13)	138.39(17)
C(12)-H(12)	101.7(16)
C(13)-H(13)	96.9(15)
C(14)-C(19)	139.46(16)
C(14)-C(15)	139.48(15)
C(15)-C(16)	138.75(16)
C(15)-H(15)	94.9(15)
C(16)-C(17)	137.41(18)
C(16)-H(16)	98.8(16)
C(17)-C(18)	138.86(18)
C(17)-H(17)	89.3(16)
C(18)-C(19)	138.82(17)
C(18)-H(18)	99.3(18)
C(19)-H(19)	91.3(16)

C(8)-P(1)-C(3)	103.33(5)

C(8)-P(1)-C(2)	96.61(5)
C(3)-P(1)-C(2)	99.93(5)
C(14)-P(2)-C(4)	103.95(5)
C(14)-P(2)-C(1)#1	95.90(5)
C(4)-P(2)-C(1)#1	100.91(5)
C(1)-N(1)-C(2)	110.30(9)
C(1)-N(1)-C(5)	112.28(9)
C(2)-N(1)-C(5)	113.15(8)
N(1)-C(1)-P(2)#1	113.90(8)
N(1)-C(1)-H(1A)	111.5(9)
P(2)#1-C(1)-H(1A)	104.8(9)
N(1)-C(1)-H(1B)	111.8(8)
P(2)#1-C(1)-H(1B)	105.3(8)
H(1A)-C(1)-H(1B)	109.2(12)
N(1)-C(2)-P(1)	111.84(7)
N(1)-C(2)-H(2A)	108.4(8)
P(1)-C(2)-H(2A)	107.9(8)
N(1)-C(2)-H(2B)	115.9(8)
P(1)-C(2)-H(2B)	104.6(8)
H(2A)-C(2)-H(2B)	107.8(11)
C(4)-C(3)-P(1)	112.52(8)
C(4)-C(3)-H(3A)	110.7(8)
P(1)-C(3)-H(3A)	106.0(8)
C(4)-C(3)-H(3B)	109.2(8)
P(1)-C(3)-H(3B)	110.4(8)
H(3A)-C(3)-H(3B)	107.9(11)
C(3)-C(4)-P(2)	110.87(8)

C(3)-C(4)-H(4A)	112.6(8)
P(2)-C(4)-H(4A)	109.1(9)
C(3)-C(4)-H(4B)	109.2(8)
P(2)-C(4)-H(4B)	106.5(8)
H(4A)-C(4)-H(4B)	108.3(12)
N(1)-C(5)-C(6)	110.26(12)
N(1)-C(5)-C(7)	114.26(12)
C(6)-C(5)-C(7)	112.11(17)
N(1)-C(5)-H(5)	105.2(8)
C(6)-C(5)-H(5)	106.4(8)
C(7)-C(5)-H(5)	108.0(8)
C(5)-C(6)-H(6A)	108.8(8)
C(5)-C(6)-H(6B)	109.5(8)
H(6A)-C(6)-H(6B)	107.8(9)
C(5)-C(6)-H(6C)	110.5(9)
H(6A)-C(6)-H(6C)	109.6(10)
H(6B)-C(6)-H(6C)	110.5(10)
C(5)-C(7)-H(7A)	108.2(8)
C(5)-C(7)-H(7B)	108.0(8)
H(7A)-C(7)-H(7B)	108.3(10)
C(5)-C(7)-H(7C)	110.9(9)
H(7A)-C(7)-H(7C)	110.7(10)
H(7B)-C(7)-H(7C)	110.6(10)
C(13)-C(8)-C(9)	117.75(10)
C(13)-C(8)-P(1)	116.96(8)
C(9)-C(8)-P(1)	125.29(8)
C(10)-C(9)-C(8)	121.00(11)

C(10)-C(9)-H(9)	117.6(9)
C(8)-C(9)-H(9)	121.4(9)
C(11)-C(10)-C(9)	120.27(12)
C(11)-C(10)-H(10)	118.8(9)
C(9)-C(10)-H(10)	120.9(10)
C(10)-C(11)-C(12)	119.60(11)
C(10)-C(11)-H(11)	120.8(9)
C(12)-C(11)-H(11)	119.5(9)
C(13)-C(12)-C(11)	119.98(11)
C(13)-C(12)-H(12)	117.8(9)
C(11)-C(12)-H(12)	122.2(9)
C(12)-C(13)-C(8)	121.38(11)
C(12)-C(13)-H(13)	119.8(9)
C(8)-C(13)-H(13)	118.7(9)
C(19)-C(14)-C(15)	118.19(10)
C(19)-C(14)-P(2)	126.17(8)
C(15)-C(14)-P(2)	115.62(9)
C(16)-C(15)-C(14)	121.13(11)
C(16)-C(15)-H(15)	119.5(9)
C(14)-C(15)-H(15)	119.4(9)
C(17)-C(16)-C(15)	119.91(11)
C(17)-C(16)-H(16)	119.7(9)
C(15)-C(16)-H(16)	120.3(10)
C(16)-C(17)-C(18)	120.08(12)
C(16)-C(17)-H(17)	120.1(10)
C(18)-C(17)-H(17)	119.7(10)
C(19)-C(18)-C(17)	119.99(12)

C(19)-C(18)-H(18)	122.7(10)
C(17)-C(18)-H(18)	117.3(10)
C(18)-C(19)-C(14)	120.68(11)
C(18)-C(19)-H(19)	117.7(10)
C(14)-C(19)-H(19)	121.6(10)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+1/2

Table S11. Anisotropic displacement parameters ($pm^2 x\ 10^{-1}$). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	17(1)	22(1)	18(1)	2(1)	5(1)	0(1)
P(2)	16(1)	23(1)	18(1)	1(1)	4(1)	0(1)
N(1)	14(1)	20(1)	21(1)	2(1)	4(1)	-1(1)
C(1)	16(1)	27(1)	21(1)	-4(1)	6(1)	-1(1)
C(2)	16(1)	25(1)	20(1)	5(1)	5(1)	0(1)
C(3)	20(1)	26(1)	19(1)	3(1)	8(1)	4(1)
C(4)	26(1)	26(1)	18(1)	3(1)	7(1)	2(1)
C(5)	19(1)	23(1)	47(1)	10(1)	9(1)	2(1)
C(6)	45(1)	27(1)	121(2)	-19(1)	-7(1)	-2(1)
C(7)	52(1)	71(1)	90(2)	62(1)	42(1)	30(1)
C(8)	18(1)	17(1)	20(1)	3(1)	6(1)	2(1)
C(9)	20(1)	27(1)	26(1)	-4(1)	5(1)	1(1)
C(10)	19(1)	28(1)	39(1)	1(1)	4(1)	0(1)
C(11)	21(1)	26(1)	45(1)	10(1)	15(1)	5(1)
C(12)	33(1)	28(1)	32(1)	6(1)	17(1)	10(1)
C(13)	26(1)	22(1)	21(1)	1(1)	7(1)	4(1)
C(14)	13(1)	25(1)	19(1)	2(1)	5(1)	0(1)
C(15)	23(1)	26(1)	21(1)	-2(1)	4(1)	2(1)
C(16)	23(1)	37(1)	19(1)	1(1)	3(1)	3(1)
C(17)	23(1)	34(1)	24(1)	10(1)	4(1)	1(1)
C(18)	35(1)	24(1)	30(1)	3(1)	6(1)	-3(1)
C(19)	30(1)	26(1)	21(1)	-1(1)	3(1)	-2(1)

Table S12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (pm^2x 10^{-1})

	x	y	z	U(eq)
H(1A)	5421(7)	145(19)	4537(8)	39(4)
H(1B)	5231(6)	1426(17)	3948(6)	26(3)
H(2A)	4051(6)	-1634(17)	3369(6)	26(3)
H(2B)	4166(7)	-358(17)	3975(7)	31(4)
H(3A)	4438(6)	-219(16)	2308(6)	21(3)
H(3B)	3686(7)	-810(18)	2159(7)	30(4)
H(4A)	4122(7)	2354(19)	1740(7)	37(4)
H(4B)	3364(7)	1846(17)	1664(6)	28(3)
H(5)	5676(7)	-2669(16)	3991(6)	23(3)
H(6A)	4463(5)	-3983(19)	3342(7)	82(7)
H(6B)	5111(7)	-4928(13)	3529(7)	86(7)
H(6C)	4993(8)	-3579(19)	3013(5)	118(11)
H(7A)	4597(5)	-3110(20)	4462(7)	96(8)
H(7B)	5232(8)	-4106(15)	4676(6)	80(6)
H(7C)	5235(9)	-2278(18)	4854(6)	141(14)
H(9)	2720(7)	-229(18)	2198(7)	30(4)
H(10)	1651(8)	-240(20)	2262(8)	43(4)
H(11)	1445(7)	944(17)	3153(7)	28(4)
H(12)	2269(8)	2300(20)	3971(8)	46(4)
H(13)	3329(7)	2360(18)	3853(7)	34(4)
H(15)	3189(7)	299(19)	-397(7)	29(4)
H(16)	2858(8)	2170(20)	-1254(8)	44(4)

H(17)	2930(7)	4940(20)	-1002(8)	39(4)
H(18)	3304(8)	5980(20)	14(8)	52(5)
H(19)	3634(7)	4070(20)	853(7)	37(4)