Supplementary Information

Recognition Between V- and Dumbbell-Shaped Molecules

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Table of Contents

Section A. NMR Characterisation

1) 2-D NOESY spectra

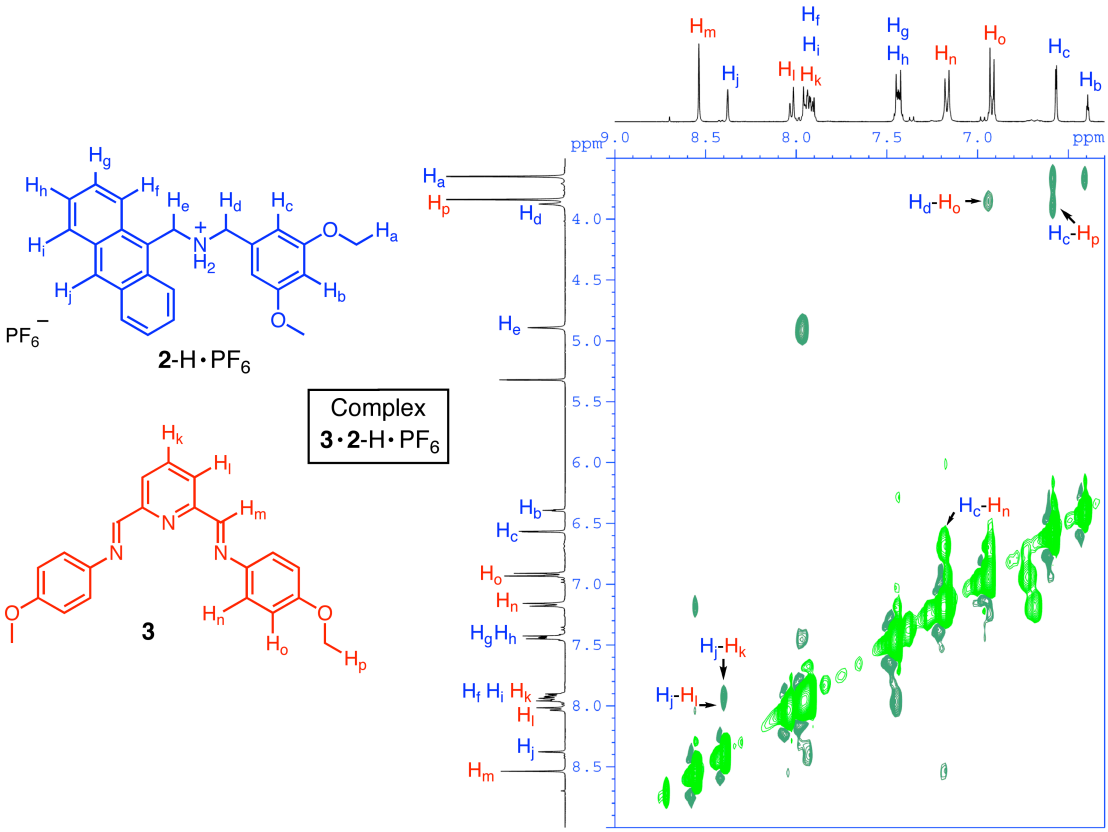


Figure S1. 2D-NOESY spectrum of equilibrating mixture of the V-shaped compound **3** and dumbbell **2**-H·PF_6 in 1:1 ratio.

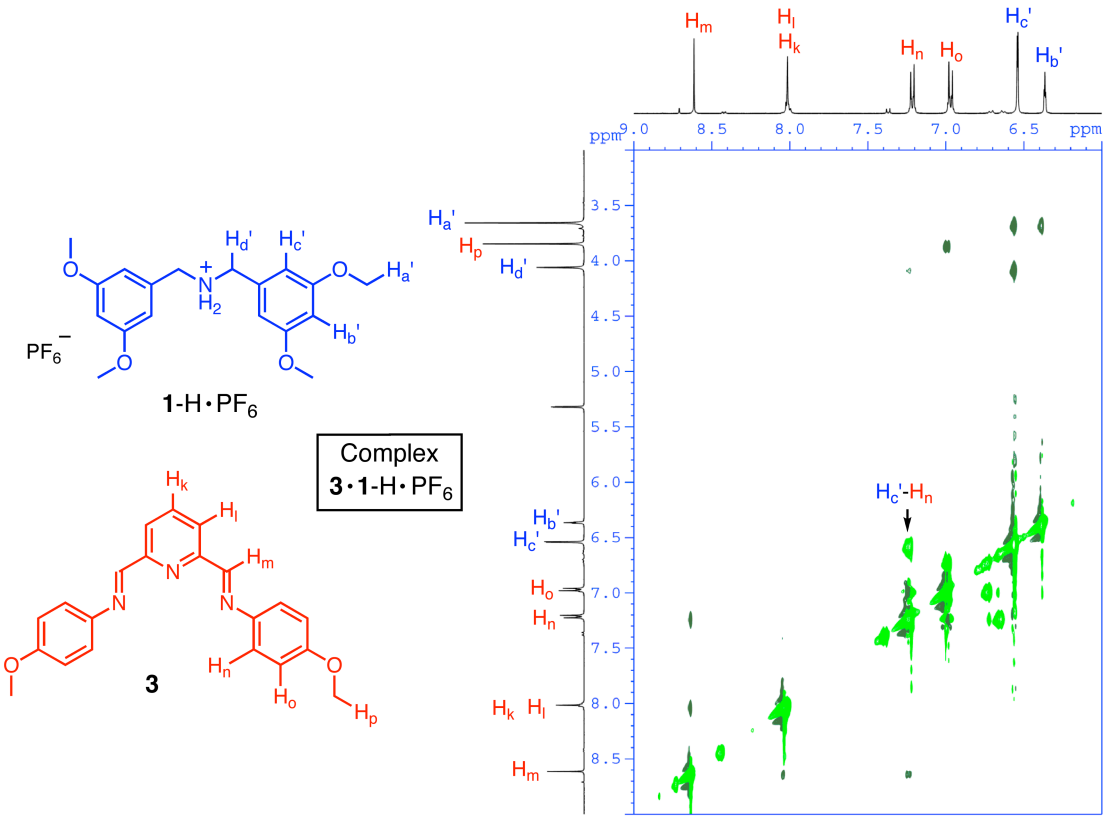


Figure S2. 2D-NOESY spectrum of equilibrating mixture of the V-shaped compound **3** and dumbbell **1**-H·PF_6 in 1:1 ratio.

2) Stacked ^{1}H NMR spectra

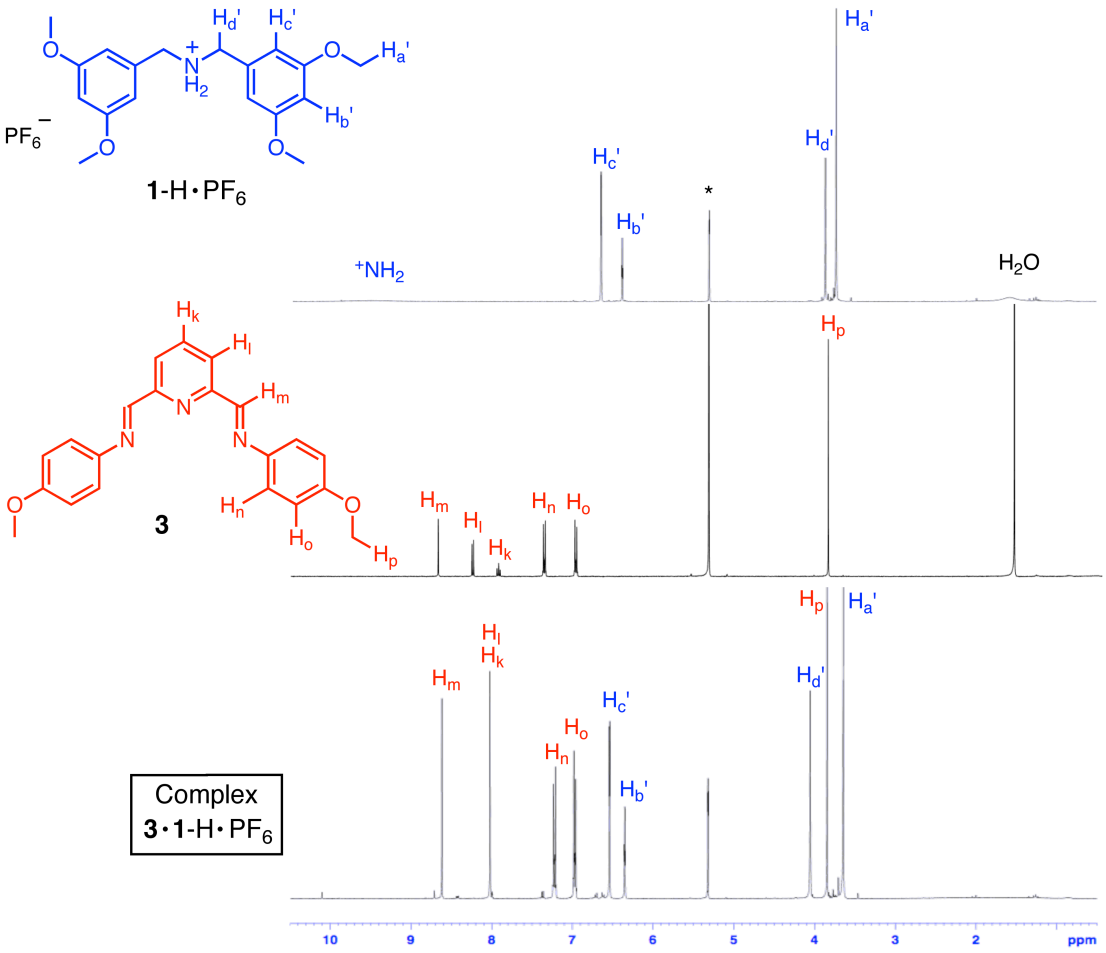


Figure S3. Stacked partial ^{1}H NMR spectra of the dumbbell **1**-H·PF_6, the V-shaped compound **3** and their equimolar mixture in CD_2Cl_2. Asterisk denotes the solvent residual signal.

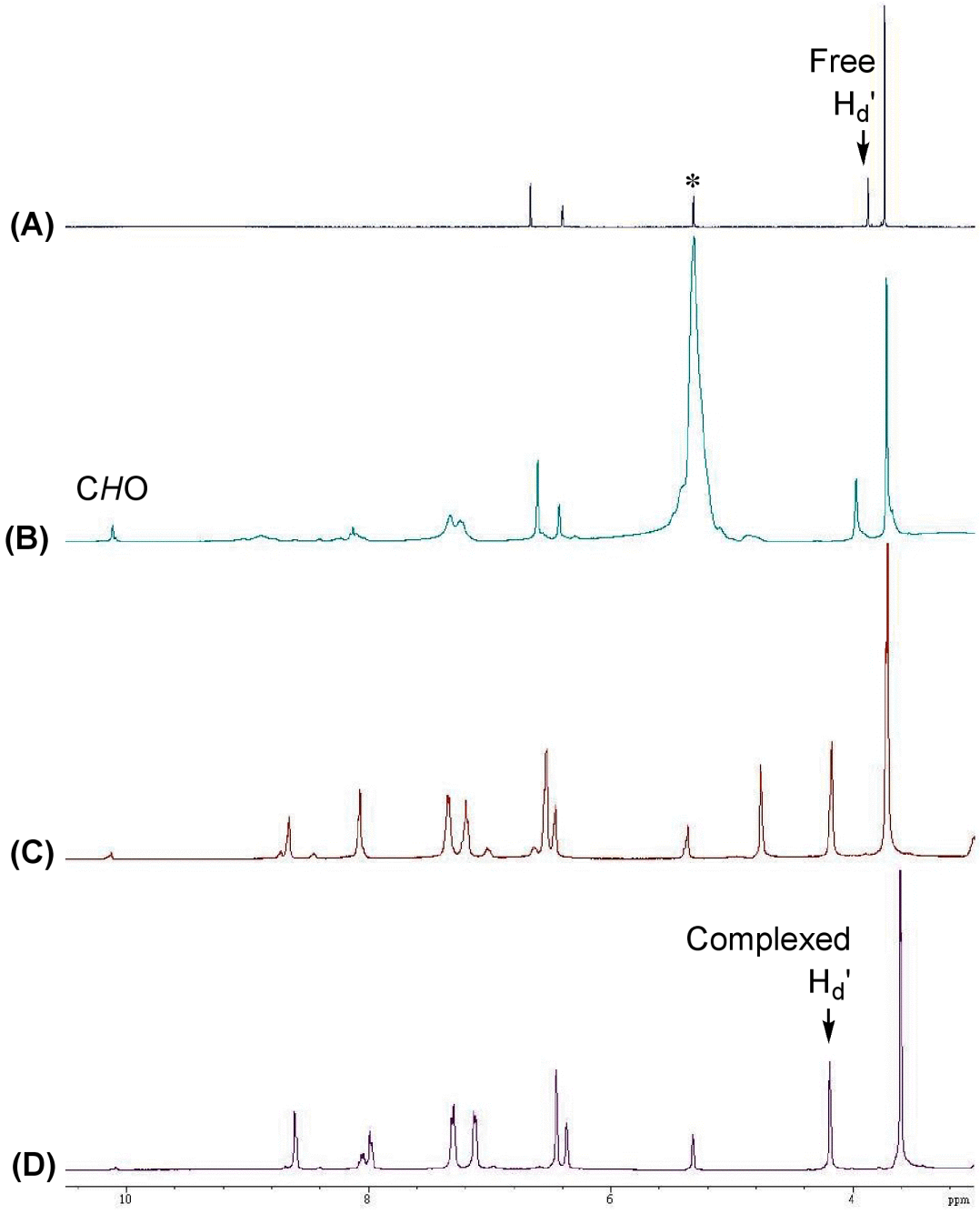


Figure S4. Stacked partial ^{1}H NMR spectra of (A) the ammonium dumbbell **1**-H·PF_6; (B) complex **4·1**-H·PF_6 with acid; (C) complex **4·1**-H·PF_6 with water; and (D) complex **4·1**-H·PF_6 in CD_2Cl_2/CD_3CN (9:1). Asterisk denotes the solvent residual signal.

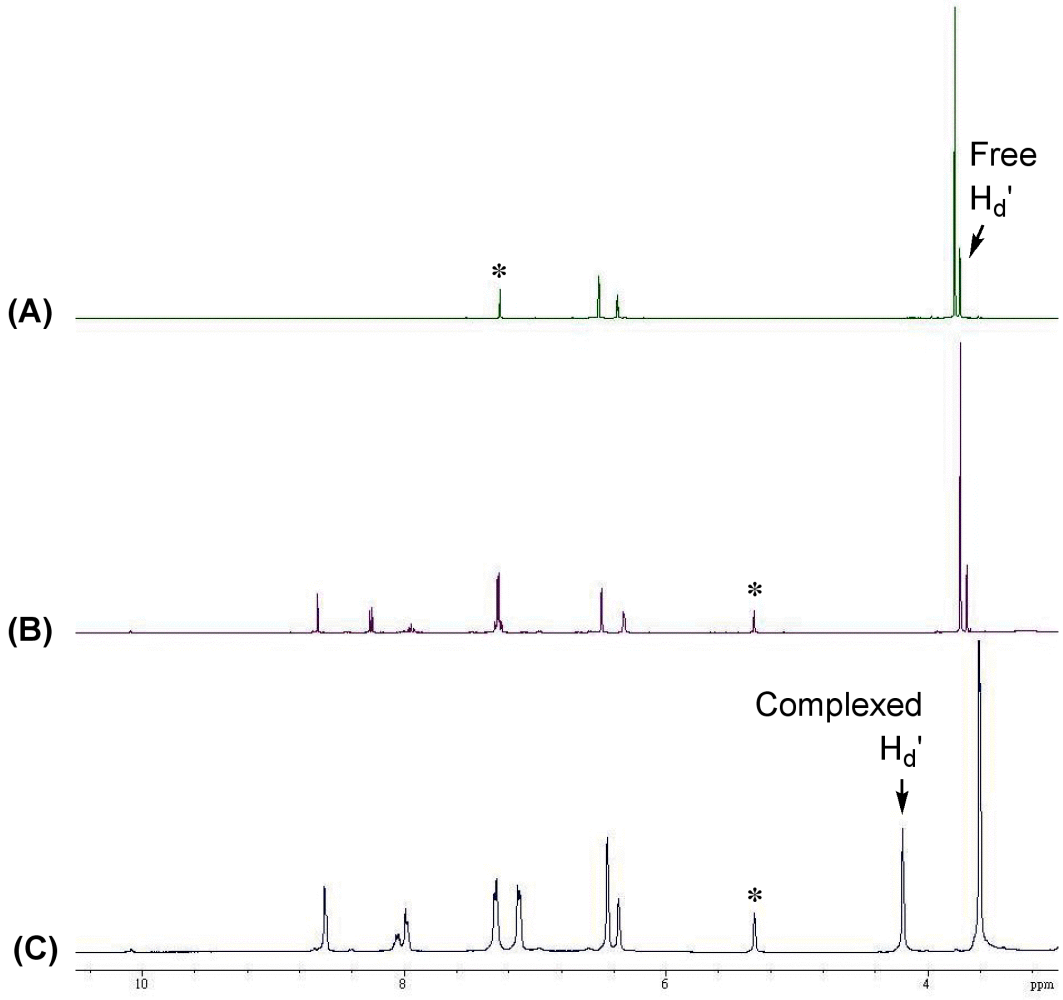


Figure S5. Stacked partial ^{1}H NMR spectra of (A) the amine dumbbell **1** in $CDCl_3$; (B) the complex **4·1**-H·PF_6 treated with base; and (C) the complex **4·1**-H·PF_6 in CD_2Cl_2/CD_3CN (9:1). Asterisk denotes the solvent residual signal.

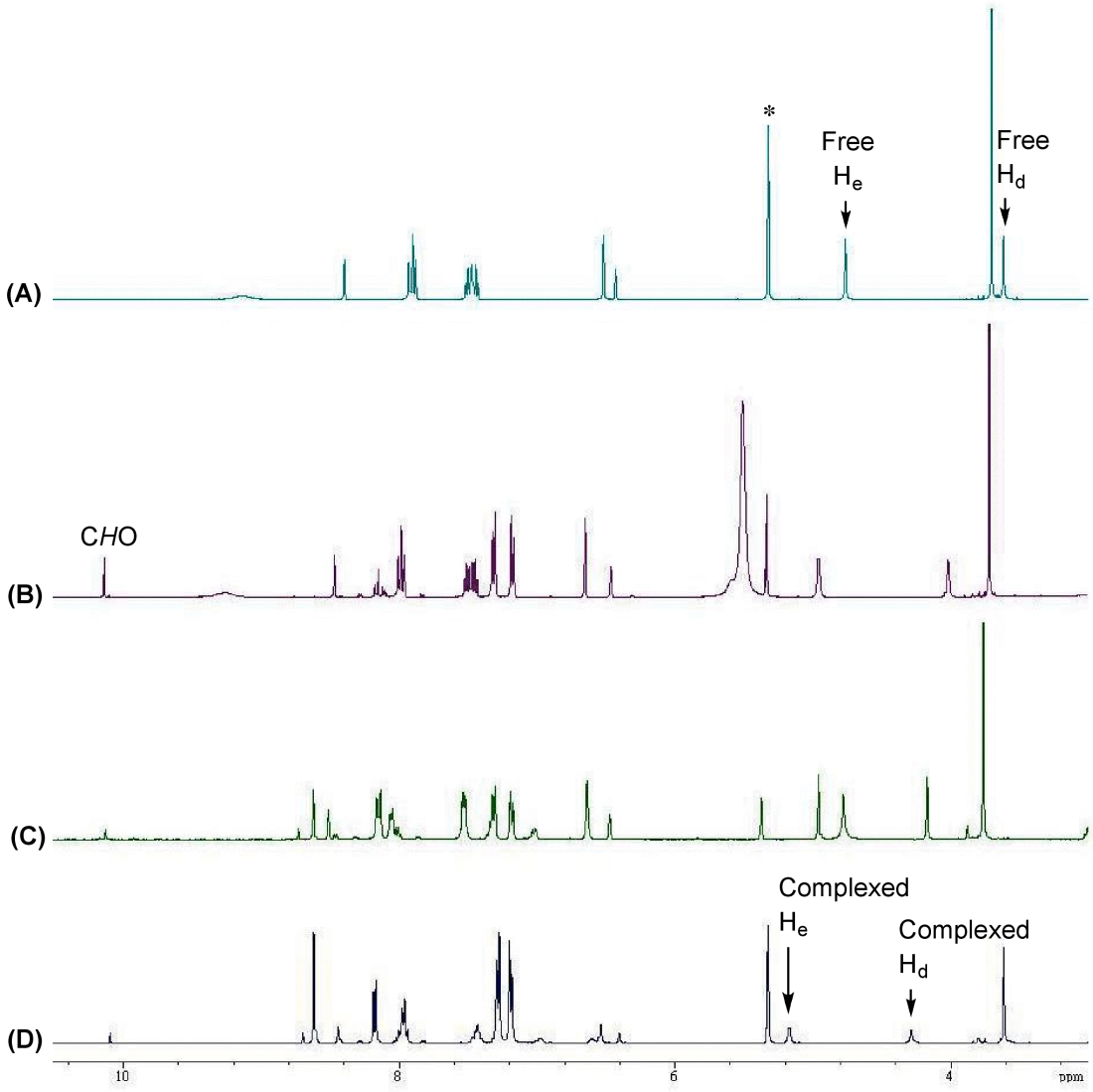


Figure S6. Stacked partial ^{1}H NMR spectra of (A) the ammonium dumbbell **2**-H·PF_6; (B) the complex **4·2**-H·PF_6 treated with acid; (C) the complex **4·2**-H·PF_6 treated with water; and (D) the complex **4·2**-H·PF_6 in CD_2Cl_2/CD_3CN (9:1). Asterisk denotes the solvent residual signal.

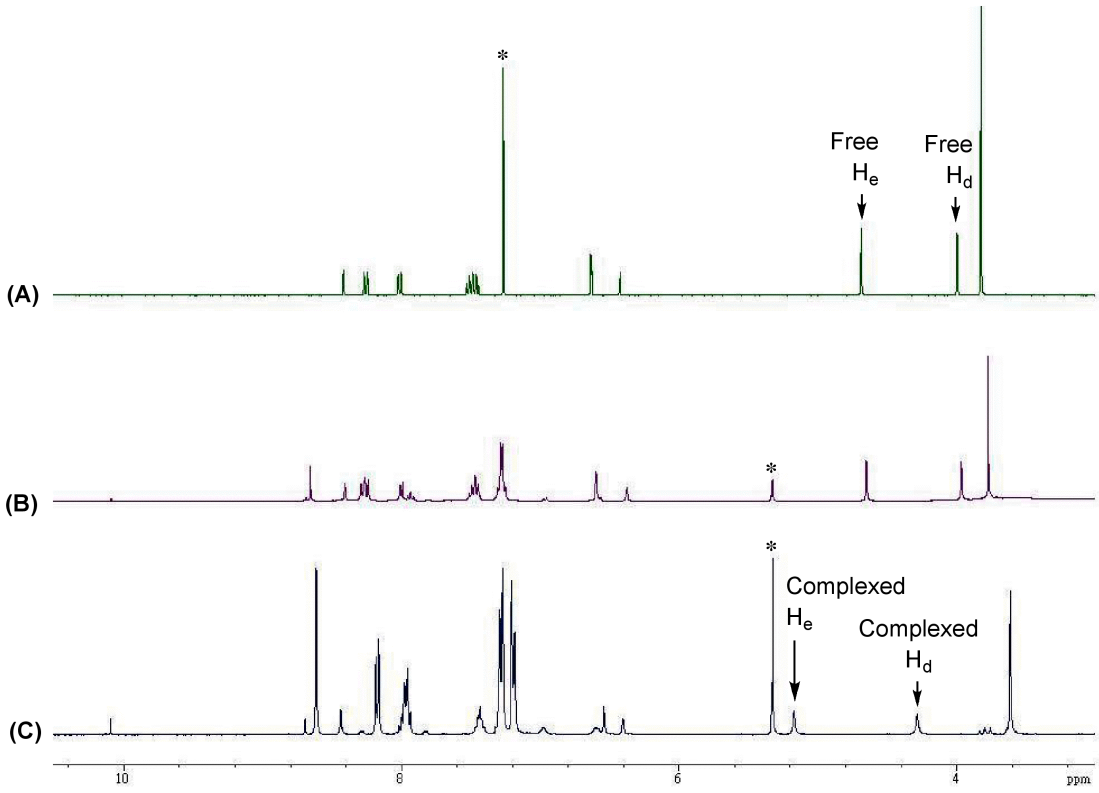
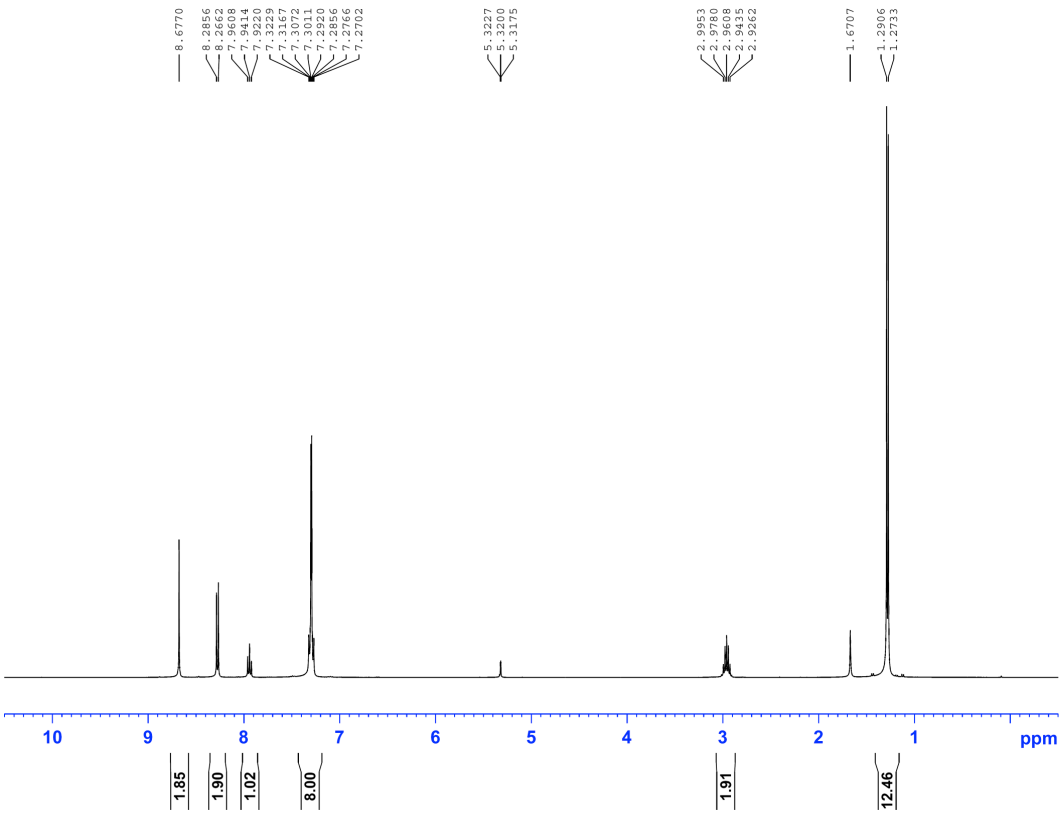


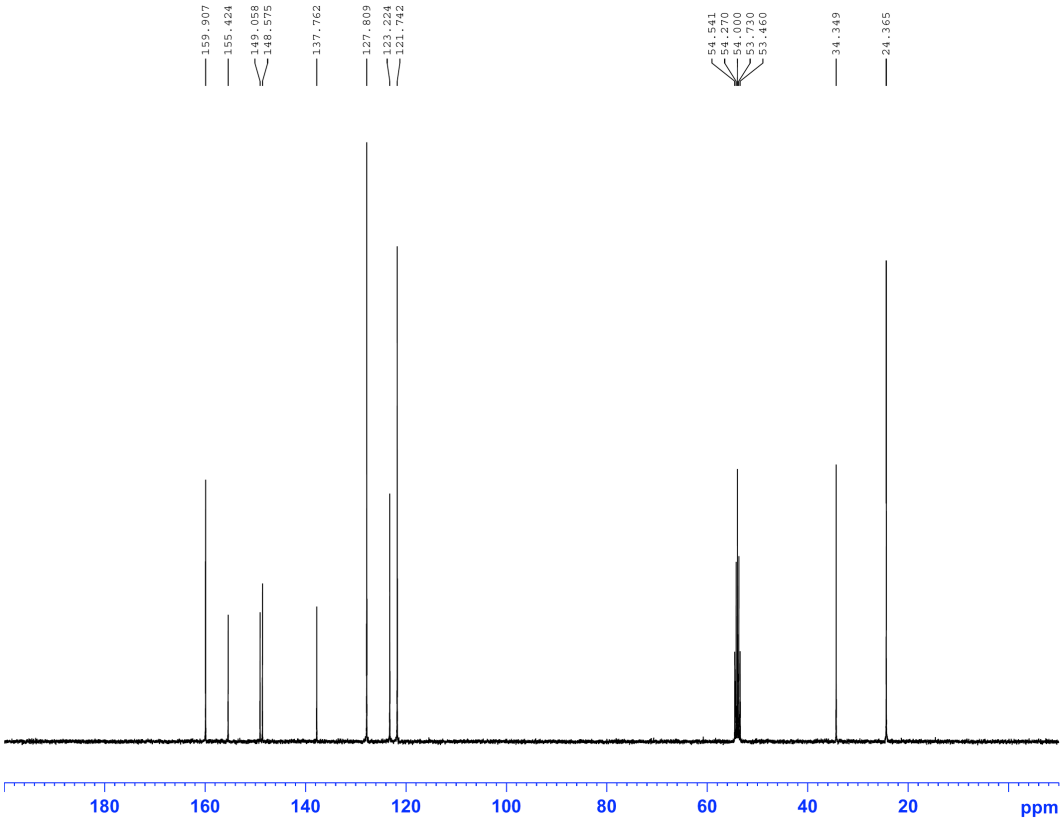
Figure S7. Stacked partial ^{1}H NMR spectra of (A) the amine dumbbell **2** in $CDCl_3$; (B) the complex **4**·**2**-H·PF_6 treated with base in CD_2Cl_2; and (C) the complex **4**·**2**-H·PF_6 in CD_2Cl_2/CD_3CN (9:1). Asterisk denotes the solvent residual signal.

3) Full ^{1}H and ^{13}C NMR Spectra

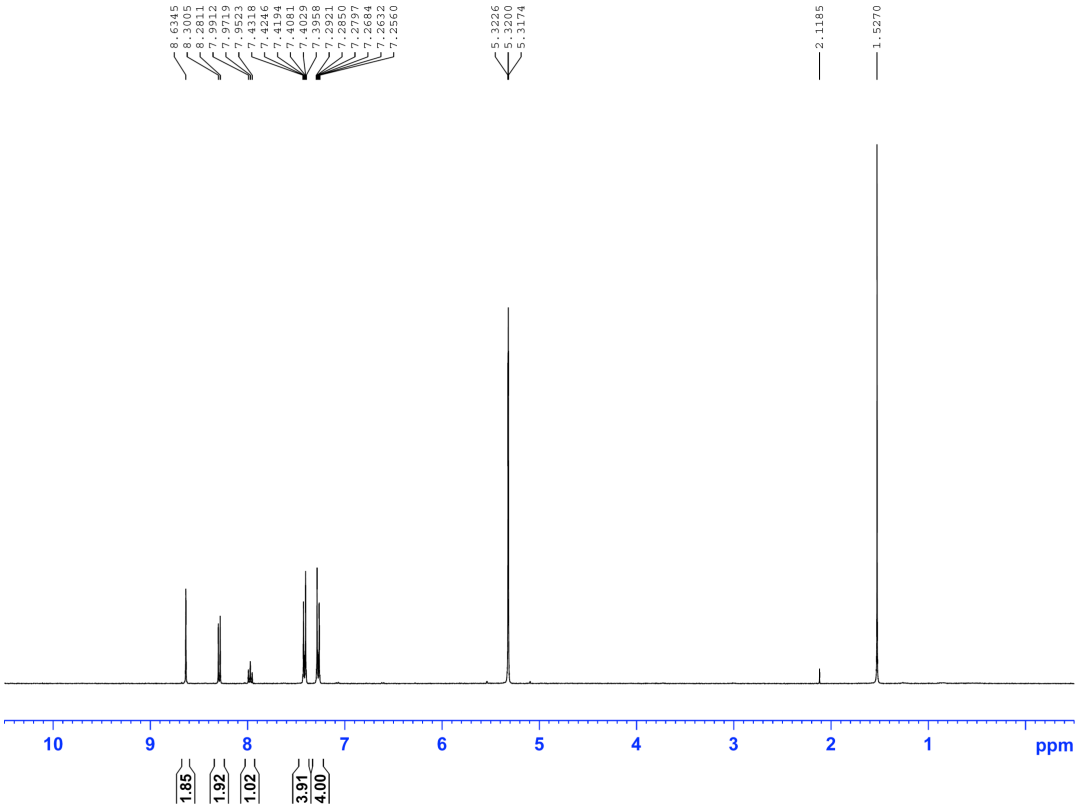
^{1}H NMR Spectrum of **4** recorded in CD_2Cl_2



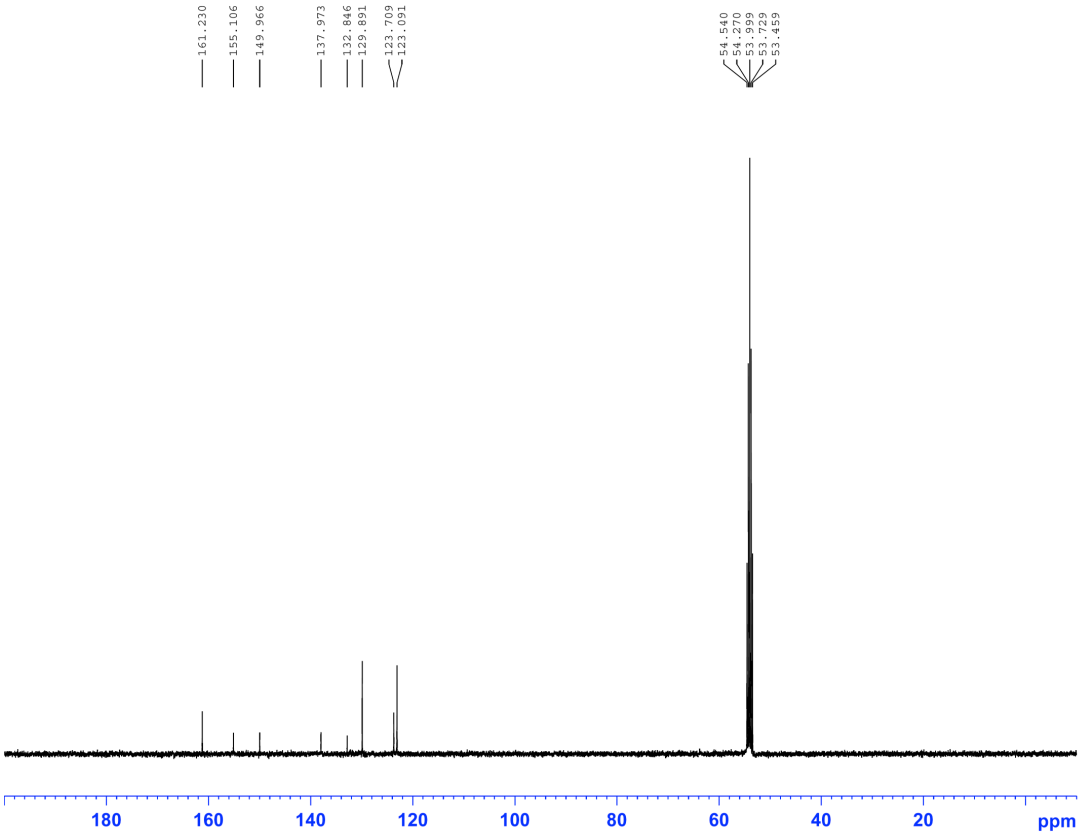
^{13}C NMR Spectrum of **4** recorded in CD_2Cl_2



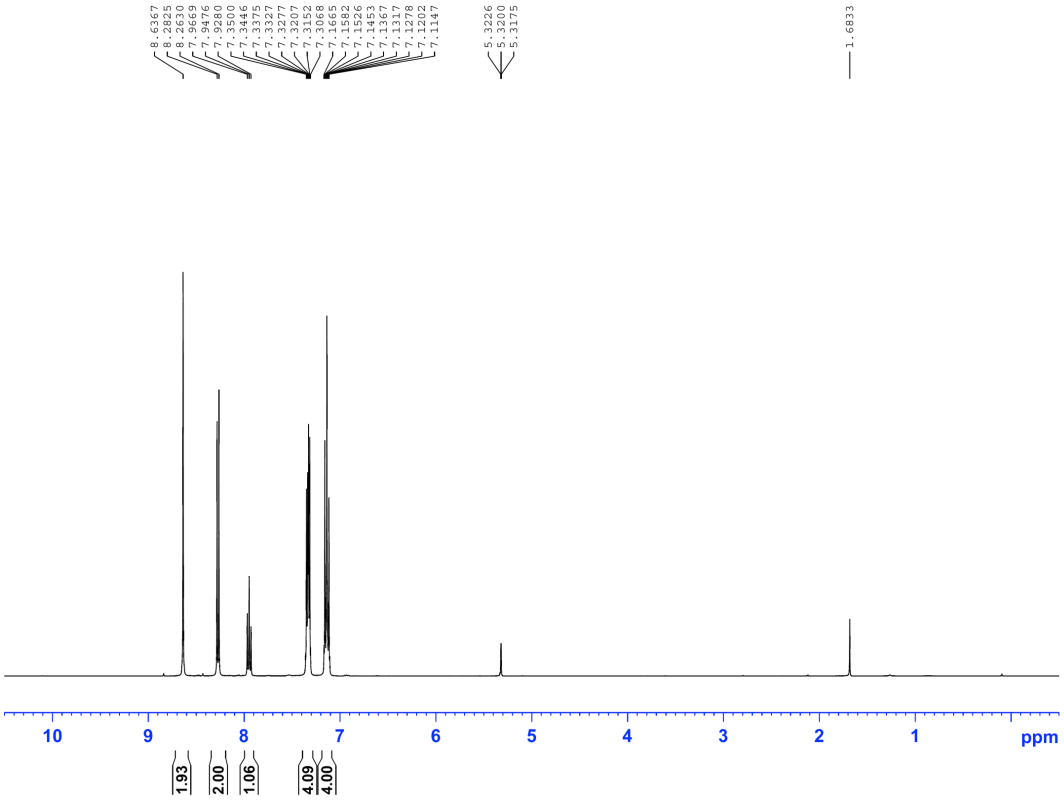
^{1}H NMR Spectrum of **7** recorded in CD_2Cl_2



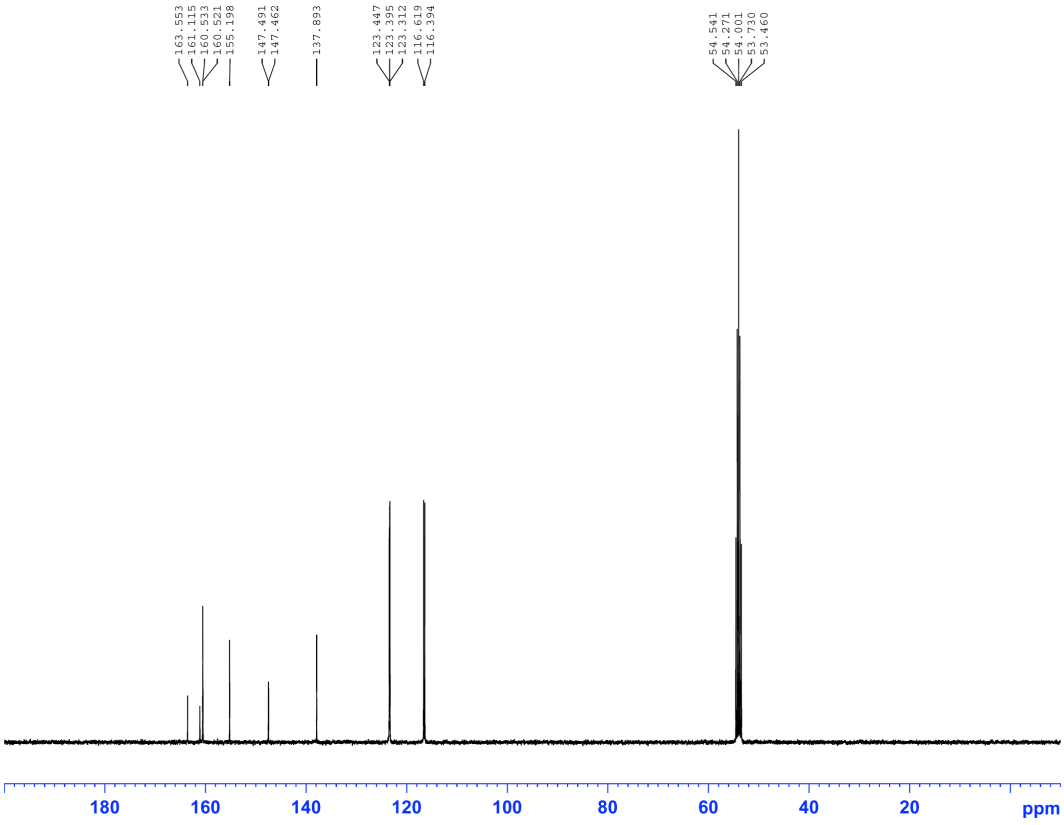
^{13}C NMR Spectrum of **7** recorded in CD_2Cl_2



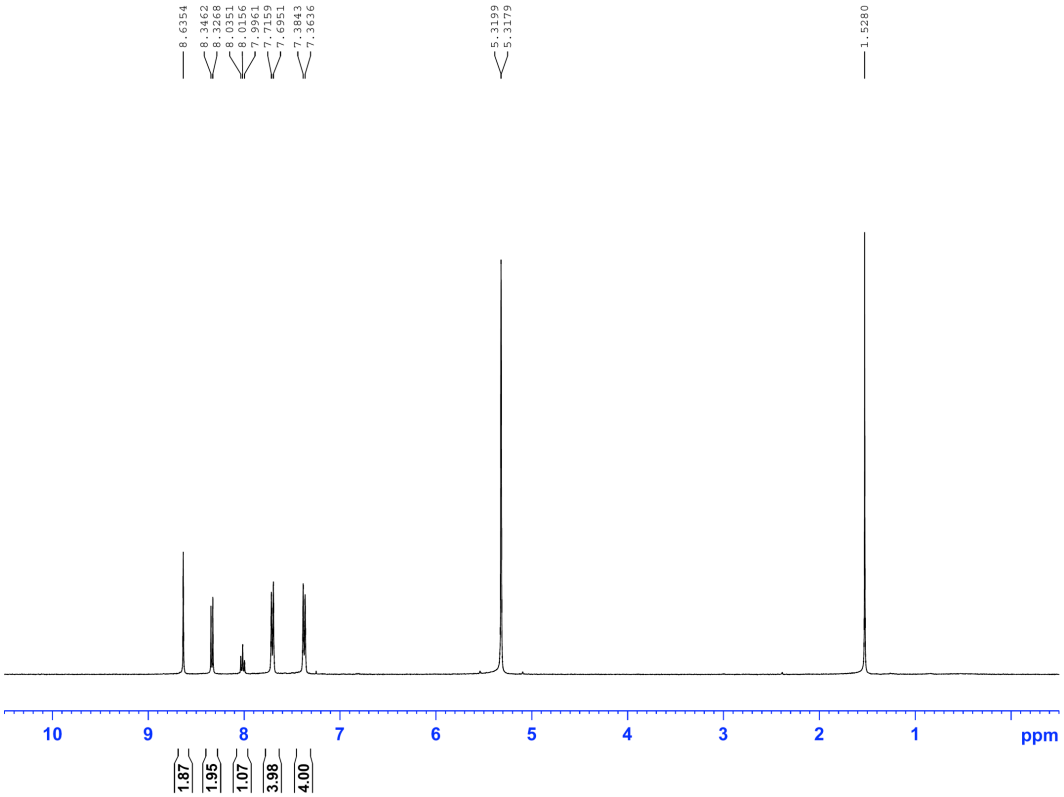
^{1}H NMR Spectrum of **8** recorded in CD_2Cl_2



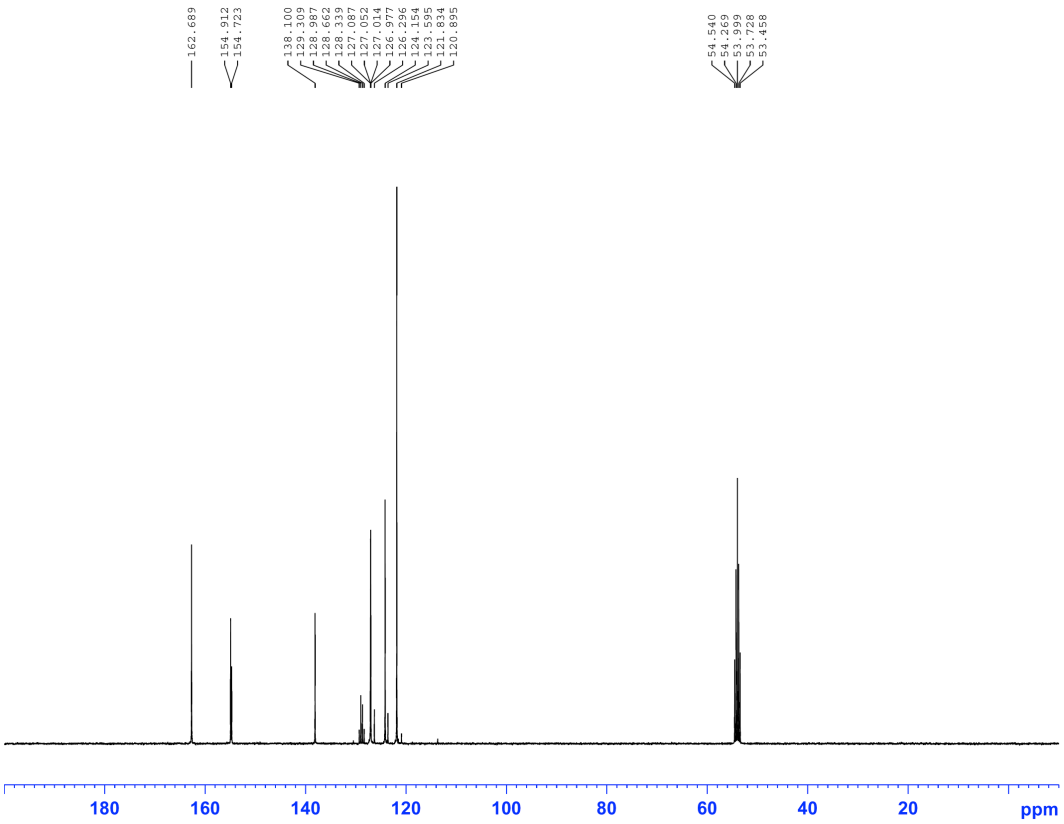
^{13}C NMR Spectrum of **8** recorded in CD_2Cl_2



^{1}H NMR Spectrum of **9** recorded in CD_2Cl_2



^{13}C NMR Spectrum of **9** recorded in CD_2Cl_2



4) Summary of Data

Table S1. Summary of K_a (M^{-1}) and δ_c (ppm) for complexes formed between the V-shaped compounds **3**–**6** and **8** and the dumbbells **1**-H·PF_6 and **2**-H·PF_6 at 295 K in CD_2Cl_2 (error = ± 1 %; n.a. = not available due to fast exchange complexation).

V-shaped molecule	**1**-H·PF_6		**2**-H·PF_6	
	binding constant K_a (M^{-1})	chemical shift of complexed dumbbell δ_c	binding constant K (M^{-1})	chemical shift of complexed dumbbell δ_c
3	n.a.	n.a.	240	5.04
4	400	4.13	180	5.04
5	360	4.10	n.a.	n.a.
6	130	4.19	n.a.	n.a.
8	90	4.13	n.a.	n.a.

Table S2. Summary of the mass-to-charge (*m/z*) ratios for the complexes formed between the V-shaped compounds **3**–**9** and the dumbbells **1**-H·PF_6 and **2**-H·PF_6 in ESI-MS.

molecular ion	calculated	found
[**3**·**1**-H]$^+$	663.3177	663.3184
[**4**·**1**-H]$^+$	687.3905	687.3922
[**5**·**1**-H]$^+$	631.3279	631.3286
[**6**·**1**-H]$^+$	603.2966	603.2961
[**7**·**1**-H]$^+$	671.2186	671.2185
[**8**·**1**-H]$^+$	639.2777	639.2771
[**9**·**1**-H]$^+$	739.2714	739.2713
[**3**·**2**-H]$^+$	703.3279	703.3294
[**4**·**2**-H]$^+$	727.4007	727.3995
[**5**·**2**-H]$^+$	671.3381	671.3376
[**6**·**2**-H]$^+$	643.3068	643.3067
[**7**·**2**-H]$^+$	711.2288	711.2312
[**8**·**2**-H]$^+$	679.2879	679.2886
[**9**·**2**-H]$^+$	779.2815	779.2826

Section B. Determination of Binding Constant

1) Job plot

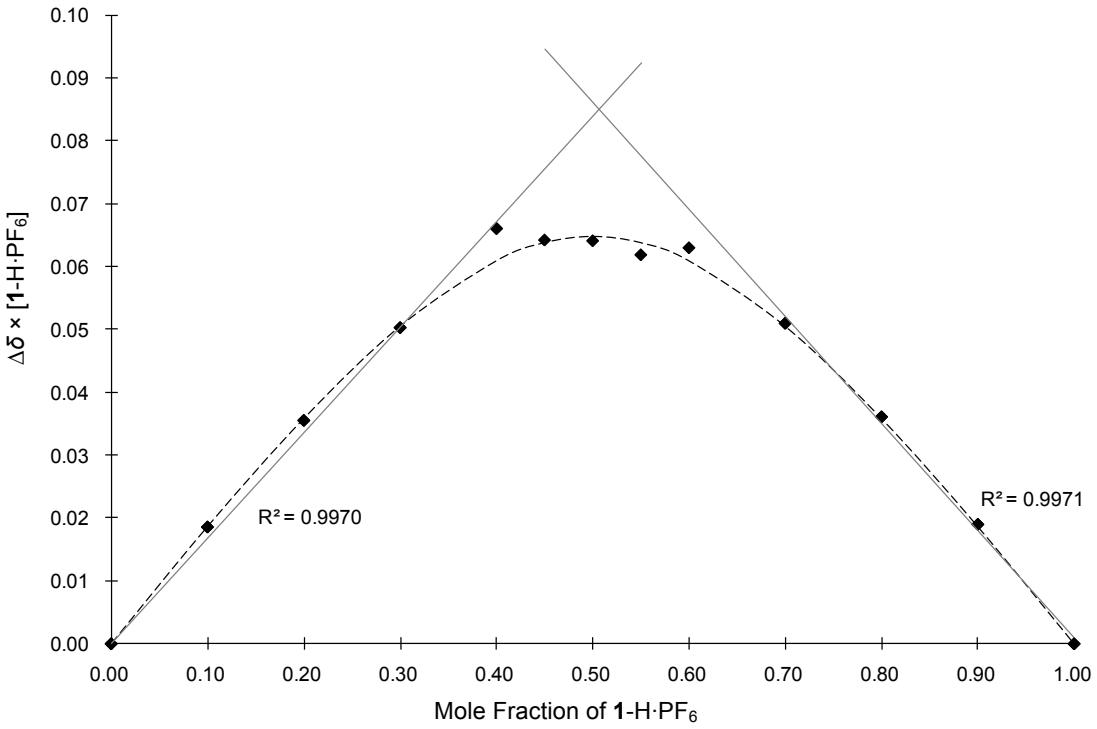


Figure S8. Job plot for complexation between V-shaped compound **5** and the dumbbell **1**-H·PF_6 (total conc = 20 mM) based on NMR spectroscopic data (♦: observed; – – – : calcd).

2) Calculation of Binding Constant

With regard to the ^{1}H NMR spectroscopic method, the binding constant determination is classified into two categories—slow and fast exchanges, depending on the rate of equilibrium relative to NMR timescale. For slow-exchange equilibria, free and complexed hosts give separate signals. The stoichiometry, concentration of complex [C] and binding constant *K* can be calculated from peak integrations. For a rapidly exchanging system, free and complexed hosts appear as a weighted average. The stoichiometry can be determined from Job plot. A titration experiment and regression (Rose-Drago method) are required to evaluate [C]. Then, *K* can be calculated by curve-fitting.

For a host-guest complexation:

$a \cdot \mathrm{H} + b \cdot \mathrm{G} \rightleftharpoons \mathrm{C}$ where H = Host, G = Guest, C = complex

$$K = \frac{[\mathrm{C}]}{[\mathrm{H}]^a \cdot [\mathrm{G}]^b} \quad \ldots(1)$$

$$[\mathrm{H}]_0 = [\mathrm{H}] + a \cdot [\mathrm{C}] \quad \ldots(2)$$

$$[\mathrm{G}]_0 = [\mathrm{G}] + b \cdot [\mathrm{C}] \quad \ldots(3)$$

K: Binding constant

a, *b*: Stoichiometry

$[\mathrm{H}]_0$: Initial (total) concentration of host molecule

$[\mathrm{G}]_0$: Initial (total) concentration of guest molecule

[H], [G], [C]: equilibrium concentrations of host, guest, and complex, respectively

Substitution of (2), (3) into (1) gives

$$K = \frac{[C]}{([H]_0 - a\cdot[C])^a \cdot ([G]_0 - b\cdot[C])^b} \quad \ldots(4)$$

For a fast-exchange equilibrium on NMR timescale

$$[H]_0 \cdot (\delta_{obs} - \delta_h) = a \cdot [C] \cdot (\delta_c - \delta_h) \quad \ldots(5)$$

where δ_{obs} = observed chemical shift

δ_h = chemical shift of free host

δ_c = chemical shift of complexed host

The stoichiometry is determined from the *x*-coordinate at the maximum in the Job plot where $[H]_0 \cdot (\delta_{obs} - \delta_h)$ is plotted against mole fraction of host $\left(\frac{[H]_0}{[H]_0 + [G]_0}\right)$.

To evaluate the complex concentration [C], simple transformation of (5) gives

$$[C] = \frac{1}{a} \cdot \frac{\delta_{obs} - \delta_h}{\delta_c - \delta_h} \cdot [H]_0 \quad \ldots(6)$$

Rose-Drago method is applied using a 1:1 complexation model ($a = b = 1$). Substitution of (6) into (4) gives

$$\frac{1}{K} = \frac{(\delta_{obs} - \delta_h)\cdot[H]_0}{(\delta_c - \delta_h)} - ([H]_0 + [G]_0) + \frac{(\delta_c - \delta_h)}{(\delta_{obs} - \delta_h)} \cdot [G]_0 \quad \ldots(7)$$

From ^{1}H NMR titration experiment with *n* different combinations of $[H]_0$ and $[G]_0$, a matrix of $\{ \delta_{obs}, [H]_{0n}, [G]_{0n} \}$ with 3 elements was obtained in which

δ_{obs} = observed chemical shift

$[H]_{0n}$ = initial concentration of host molecule for *n*-th measurement

$[G]_{0n}$ = initial concentration of guest molecule for *n*-th measurement

Using the following definitions:

$$Y = \frac{1}{K}$$

$$X = (\delta_{obs} - \delta_h)$$

$$a_n = [\mathrm{H}]_{0n} \cdot (\delta_{obs\,n} - \delta_h)$$

$$b_n = [\mathrm{H}]_{0n} + [\mathrm{G}]_{0n}$$

$$c_n = \frac{[\mathrm{G}]_{0n}}{\delta_{obs\,n} - \delta_h}$$

(7) is then expressed as $Y = \frac{a_n}{X} - b_n + c_n \cdot X$

A combination of data gives a matrix of answers { X, Y }. The maximum numbers of obtainable answer pairs { X, Y } is ${}_nC_2$ pairs for n combinations of concentration conditions. The binding constant K and chemical shift of complexed host δ_c can then be obtained. Values differed by more than 2.5 standard deviations from the mean are eliminated and a new mean is determined. The calculated K and δ_c are fitted back into the Job plot for optimization.

Section C. X-Ray Crystal Data

Crystal Data of the ammonium dumbbell **2**-H·PF_6

Table 1. Crystal data and structure refinement for p.

CCDC code	784761
Identification code	wy207
Empirical formula	$C_{48}H_{48}ClF_6N_2O_4P$
Formula weight	897.30
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, $P\bar{1}$
Unit cell dimensions	a = 12.0530(4) Å α = 95.8310(10) ° b = 12.8073(4) Å β = 99.9830(10) ° c = 16.0081(9) Å γ = 114.1490(10) °
Volume	2179.41(16) $Å^3$
Z, Calculated density	2, 1.367 Mg/m^3
Absorption coefficient	0.197 mm^{-1}
F(000)	936
Crystal size	0.50 x 0.40 x 0.30 mm
Theta range for data collection	1.32 to 25.25 °
Limiting indices	$-14 \le h \le 14$, $-15 \le k \le 15$, $-19 \le l \le 19$
Reflections collected / unique	25221 / 7855 [R_{int} = 0.0434]
Completeness to θ = 25.25	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6068
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7855 / 0 / 562
Goodness-of-fit on F^2	1.011
Final R indices [I > 2σ(I)]	R_1 = 0.0420, $_wR_2$ = 0.1117
R indices (all data)	R_1 = 0.0524, $_wR_2$ = 0.1235
Largest diff. peak and hole	0.424 and −0.327 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for p.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)		
N(1')	1202(1)	2060(1)	3018(1)			37(1)
N(1)	−1444(1)	869(1)	−508(1)			37(1)
O(1')	5916(1)	5342(1)	4176(1)			61(1)
O(2')	4352(2)	4790(1)	1159(1)			64(1)
C(1)	−971(2)	1418(2)	−1239(1)			43(1)
C(2)	−1986(2)	971(2)	−2061(1)			39(1)
C(3)	−2374(2)	1735(2)	−2444(1)			46(1)
C(4)	−3283(2)	1305(2)	−3209(1)			50(1)
C(5)	−3826(2)	131(2)	−3598(1)			45(1)
C(6)	−3433(2)	−609(2)	−3210(1)			41(1)
C(7)	−2519(2)	−193(2)	−2439(1)			42(1)
C(8)	−3163(4)	3183(3)	−3341(2)			116(1)
C(9)	−4867(2)	−2273(2)	−4293(2)			65(1)
C(10)	−2498(2)	1118(2)	−319(1)			39(1)
C(11)	−3074(2)	516(2)	363(1)			38(1)
C(12)	−3942(2)	−670(2)	130(1)			42(1)
C(13)	−4230(2)	−1354(2)	−709(2)			52(1)
C(14)	−5087(2)	−2485(2)	−914(2)			69(1)
C(15)	−5719(2)	−3020(2)	−301(2)			78(1)
C(16)	−5475(2)	−2423(2)	503(2)			67(1)
C(17)	−4586(2)	−1223(2)	752(2)			49(1)
C(18)	−4371(2)	−573(2)	1559(1)			53(1)
C(19)	−3530(2)	599(2)	1796(1)			47(1)
C(20)	−3346(2)	1281(2)	2617(1)			62(1)
C(21)	−2531(2)	2408(3)	2848(2)			69(1)
C(22)	−1830(2)	2953(2)	2270(2)			63(1)
C(23)	−1972(2)	2358(2)	1474(1)			52(1)
C(24)	−2840(2)	1158(2)	1194(1)			41(1)
C(1')	1452(2)	3314(2)	3048(1)			45(1)
C(2')	2733(2)	3985(2)	2902(1)			40(1)
C(3')	3758(2)	4415(2)	3596(1)			42(1)
C(4')	4955(2)	4957(2)	3458(1)			44(1)
C(5')	5117(2)	5078(2)	2636(1)			48(1)
C(6')	4085(2)	4646(2)	1943(1)			46(1)
C(7')	2884(2)	4103(2)	2070(1)			44(1)
C(8')	7114(2)	5535(3)	4042(2)			74(1)
C(9')	3360(2)	4169(2)	415(2)			70(1)
C(10')	91(2)	1336(2)	3351(1)			46(1)
C(11')	169(2)	235(2)	3550(1)			43(1)
C(12')	−555(2)	−844(2)	2979(1)		43(1)	
C(13')	−1469(2)	−1019(2)	2215(2)			55(1)
C(14')	−2136(2)	−2080(2)	1689(2)			63(1)
C(15')	−1931(2)	−3047(2)	1874(2)			67(1)
C(16')	−1083(2)	−2935(2)	2585(2)			60(1)

C(17')	−383(2)	−1851(2)	3170(1)		48(1)
C(18')	473(2)	−1743(2)	3914(1)	52(1)	
C(19')	1175(2)	−692(2)	4488(1)		49(1)
C(20')	2055(2)	−593(2)	5251(2)		63(1)
C(21')	2749(3)	435(3)	5796(2)		73(1)
C(22')	2610(2)	1440(2)	5625(2)		69(1)
C(23')	1787(2)	1388(2)	4914(1)		56(1)
C(24')	1028(2)	323(2)	4305(1)		46(1)
O(1)	−3733(2)	1958(2)	−3656(1)		84(1)
O(2)	−3854(2)	−1768(1)	−3543(1)		59(1)
P(1')	0	5000	5000		50(1)
P(1)	0	5000	0		68(1)
F(1')	1400(1)	5794(2)	4984(1)		86(1)
F(1)	−565(3)	5182(2)	766(2)		167(1)
F(2')	133(2)	3864(1)	4635(1)		83(1)
F(2)	1338(2)	5874(2)	512(2)		152(1)
F(3')	−472(2)	5134(1)	4045(1)		80(1)
F(3)	185(2)	3934(2)	318(2)		109(1)
Cl(1)	689(1)	1239(1)	1054(1)		53(1)

Table 3. Bond lengths [Å] and angles [°] for p.

N(1')-C(1')	1.502(2)
N(1')-C(10')	1.506(2)
N(1)-C(10)	1.501(2)
N(1)-C(1)	1.502(2)
O(1')-C(4')	1.364(2)
O(1')-C(8')	1.420(3)
O(2')-C(6')	1.361(2)
O(2')-C(9')	1.420(3)
C(1)-C(2)	1.508(3)
C(2)-C(7)	1.378(3)
C(2)-C(3)	1.396(3)
C(3)-C(4)	1.381(3)
C(4)-O(1)	1.365(2)
C(4)-C(5)	1.393(3)
C(5)-C(6)	1.376(3)
C(6)-O(2)	1.370(2)
C(6)-C(7)	1.391(3)
C(8)-O(1)	1.423(3)
C(9)-O(2)	1.427(3)
C(10)-C(11)	1.504(2)
C(11)-C(24)	1.409(3)
C(11)-C(12)	1.410(3)
C(12)-C(13)	1.430(3)
C(12)-C(17)	1.434(3)
C(13)-C(14)	1.354(3)
C(14)-C(15)	1.407(4)
C(15)-C(16)	1.347(4)
C(16)-C(17)	1.431(3)
C(17)-C(18)	1.385(3)
C(18)-C(19)	1.389(3)
C(19)-C(20)	1.431(3)
C(19)-C(24)	1.437(3)
C(20)-C(21)	1.338(4)
C(21)-C(22)	1.405(4)
C(22)-C(23)	1.362(3)
C(23)-C(24)	1.427(3)
C(1')-C(2')	1.503(3)
C(2')-C(3')	1.382(3)
C(2')-C(7')	1.390(3)
C(3')-C(4')	1.391(3)
C(4')-C(5')	1.378(3)
C(5')-C(6')	1.386(3)
C(6')-C(7')	1.388(3)
C(10')-C(11')	1.512(3)
C(11')-C(12')	1.410(3)
C(11')-C(24')	1.411(3)
C(12')-C(13')	1.427(3)
C(12')-C(17')	1.441(3)

C(13')-C(14')	1.356(3)
C(14')-C(15')	1.408(4)
C(15')-C(16')	1.342(4)
C(16')-C(17')	1.422(3)
C(17')-C(18')	1.387(3)
C(18')-C(19')	1.386(3)
C(19')-C(20')	1.430(3)
C(19')-C(24')	1.433(3)
C(20')-C(21')	1.344(4)
C(21')-C(22')	1.411(4)
C(22')-C(23')	1.350(3)
C(23')-C(24')	1.430(3)
P(1')-F(1')#1	1.5801(15)
P(1')-F(1')	1.5802(15)
P(1')-F(3')#1	1.5886(14)
P(1')-F(3')	1.5886(14)
P(1')-F(2')#1	1.5924(13)
P(1')-F(2')	1.5924(13)
P(1)-F(1)	1.543(2)
P(1)-F(1)#2	1.543(2)
P(1)-F(2)	1.5505(19)
P(1)-F(2)#2	1.5505(19)
P(1)-F(3)#2	1.5882(17)
P(1)-F(3)	1.5882(17)
C(1')-N(1')-C(10')	115.38(14)
C(10)-N(1)-C(1)	111.79(14)
C(4')-O(1')-C(8')	116.97(17)
C(6')-O(2')-C(9')	117.20(17)
N(1)-C(1)-C(2)	111.54(14)
C(7)-C(2)-C(3)	120.10(18)
C(7)-C(2)-C(1)	119.74(17)
C(3)-C(2)-C(1)	120.15(17)
C(4)-C(3)-C(2)	118.83(18)
O(1)-C(4)-C(3)	124.79(19)
O(1)-C(4)-C(5)	113.64(19)
C(3)-C(4)-C(5)	121.57(18)
C(6)-C(5)-C(4)	118.76(18)
O(2)-C(6)-C(5)	124.49(18)
O(2)-C(6)-C(7)	114.94(16)
C(5)-C(6)-C(7)	120.54(17)
C(2)-C(7)-C(6)	120.19(17)
N(1)-C(10)-C(11)	114.14(14)
C(24)-C(11)-C(12)	120.76(17)
C(24)-C(11)-C(10)	120.15(16)
C(12)-C(11)-C(10)	118.80(16)
C(11)-C(12)-C(13)	122.94(18)
C(11)-C(12)-C(17)	119.33(18)
C(13)-C(12)-C(17)	117.73(18)
C(14)-C(13)-C(12)	121.3(2)
C(13)-C(14)-C(15)	120.6(2)

C(16)-C(15)-C(14)	120.8(2)
C(15)-C(16)-C(17)	120.9(2)
C(18)-C(17)-C(16)	122.0(2)
C(18)-C(17)-C(12)	119.27(18)
C(16)-C(17)-C(12)	118.7(2)
C(17)-C(18)-C(19)	122.17(18)
C(18)-C(19)-C(20)	122.1(2)
C(18)-C(19)-C(24)	119.39(18)
C(20)-C(19)-C(24)	118.5(2)
C(21)-C(20)-C(19)	122.1(2)
C(20)-C(21)-C(22)	119.6(2)
C(23)-C(22)-C(21)	121.2(2)
C(22)-C(23)-C(24)	121.3(2)
C(11)-C(24)-C(23)	123.80(17)
C(11)-C(24)-C(19)	119.01(18)
C(23)-C(24)-C(19)	117.16(18)
N(1')-C(1')-C(2')	109.31(14)
C(3')-C(2')-C(7')	120.73(17)
C(3')-C(2')-C(1')	119.04(17)
C(7')-C(2')-C(1')	120.10(17)
C(2')-C(3')-C(4')	119.51(18)
O(1')-C(4')-C(5')	123.86(18)
O(1')-C(4')-C(3')	115.83(17)
C(5')-C(4')-C(3')	120.31(18)
C(4')-C(5')-C(6')	119.89(18)
O(2')-C(6')-C(5')	115.05(17)
O(2')-C(6')-C(7')	124.44(18)
C(5')-C(6')-C(7')	120.51(18)
C(6')-C(7')-C(2')	119.05(18)
N(1')-C(10')-C(11')	110.11(14)
C(12')-C(11')-C(24')	120.54(18)
C(12')-C(11')-C(10')	121.15(18)
C(24')-C(11')-C(10')	118.25(18)
C(11')-C(12')-C(13')	124.29(18)
C(11')-C(12')-C(17')	118.90(18)
C(13')-C(12')-C(17')	116.81(18)
C(14')-C(13')-C(12')	121.6(2)
C(13')-C(14')-C(15')	120.8(2)
C(16')-C(15')-C(14')	120.3(2)
C(15')-C(16')-C(17')	121.3(2)
C(18')-C(17')-C(16')	121.2(2)
C(18')-C(17')-C(12')	119.55(19)
C(16')-C(17')-C(12')	119.2(2)
C(19')-C(18')-C(17')	122.13(19)
C(18')-C(19')-C(20')	121.5(2)
C(18')-C(19')-C(24')	119.22(19)
C(20')-C(19')-C(24')	119.3(2)
C(21')-C(20')-C(19')	121.1(2)
C(20')-C(21')-C(22')	120.2(2)
C(23')-C(22')-C(21')	120.8(2)

C(22')-C(23')-C(24')	121.8(2)
C(11')-C(24')-C(23')	123.49(19)
C(11')-C(24')-C(19')	119.64(18)
C(23')-C(24')-C(19')	116.9(2)
C(4)-O(1)-C(8)	117.5(2)
C(6)-O(2)-C(9)	117.73(16)
F(1')#1-P(1')-F(1')	180.000(1)
F(1')#1-P(1')-F(3')#1	90.56(9)
F(1')-P(1')-F(3')#1	89.44(9)
F(1')#1-P(1')-F(3')	89.44(9)
F(1')-P(1')-F(3')	90.56(9)
F(3')#1-P(1')-F(3')	180.00(12)
F(1')#1-P(1')-F(2')#1	90.62(9)
F(1')-P(1')-F(2')#1	89.38(9)
F(3')#1-P(1')-F(2')#1	90.66(8)
F(3')-P(1')-F(2')#1	89.34(8)
F(1')#1-P(1')-F(2')	89.38(9)
F(1')-P(1')-F(2')	90.62(9)
F(3')#1-P(1')-F(2')	89.34(8)
F(3')-P(1')-F(2')	90.66(8)
F(2')#1-P(1')-F(2')	180.000(1)
F(1)-P(1)-F(1)#2	180.0
F(1)-P(1)-F(2)	91.91(18)
F(1)#2-P(1)-F(2)	88.09(18)
F(1)-P(1)-F(2)#2	88.09(18)
F(1)#2-P(1)-F(2)#2	91.91(18)
F(2)-P(1)-F(2)#2	179.999(1)
F(1)-P(1)-F(3)#2	88.23(13)
F(1)#2-P(1)-F(3)#2	91.77(13)
F(2)-P(1)-F(3)#2	88.33(11)
F(2)#2-P(1)-F(3)#2	91.67(11)
F(1)-P(1)-F(3)	91.77(13)
F(1)#2-P(1)-F(3)	88.23(13)
F(2)-P(1)-F(3)	91.67(11)
F(2)#2-P(1)-F(3)	88.33(11)
F(3)#2-P(1)-F(3)	180.0

Symmetry transformations used to generate equivalent atoms:
#1 −x, −y+1, −z+1 #2 –x, −y+1, −z

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for p.

The anisotropic displacement factor exponent takes the form:
$-2\pi^2$ [h^2 a^{*2} U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(1')	37(1)	35(1)	39(1)	7(1)	11(1)	16(1)
N(1)	31(1)	46(1)	35(1)	5(1)	5(1)	18(1)
O(1')	44(1)	78(1)	52(1)	8(1)	2(1)	23(1)
O(2')	64(1)	70(1)	46(1)	16(1)	17(1)	16(1)
C(1)	37(1)	50(1)	43(1)	9(1)	16(1)	17(1)
C(2)	40(1)	48(1)	36(1)	11(1)	18(1)	22(1)
C(3)	55(1)	39(1)	50(1)	12(1)	20(1)	22(1)
C(4)	60(1)	48(1)	53(1)	18(1)	15(1)	33(1)
C(5)	51(1)	49(1)	40(1)	11(1)	9(1)	26(1)
C(6)	51(1)	42(1)	38(1)	10(1)	15(1)	25(1)
C(7)	54(1)	49(1)	39(1)	13(1)	15(1)	33(1)
C(8)	170(4)	59(2)	119(3)	17(2)	−12(2)	68(2)
C(9)	72(2)	53(1)	58(1)	−1(1)	1(1)	24(1)
C(10)	38(1)	46(1)	41(1)	11(1)	14(1)	23(1)
C(11)	33(1)	46(1)	41(1)	13(1)	11(1)	22(1)
C(12)	34(1)	46(1)	52(1)	13(1)	9(1)	23(1)
C(13)	43(1)	52(1)	61(1)	4(1)	8(1)	23(1)
C(14)	60(1)	53(1)	86(2)	−3(1)	2(1)	28(1)
C(15)	62(2)	40(1)	121(3)	14(1)	10(2)	16(1)
C(16)	56(1)	51(1)	101(2)	34(1)	23(1)	24(1)
C(17)	39(1)	49(1)	68(1)	26(1)	16(1)	24(1)
C(18)	47(1)	70(1)	61(1)	36(1)	26(1)	33(1)
C(19)	41(1)	66(1)	45(1)	20(1)	15(1)	31(1)
C(20)	63(1)	96(2)	43(1)	21(1)	22(1)	47(1)
C(21)	68(2)	98(2)	45(1)	−2(1)	8(1)	44(2)
C(22)	53(1)	68(2)	60(1)	−7(1)	4(1)	26(1)
C(23)	43(1)	57(1)	52(1)	7(1)	12(1)	19(1)
C(24)	35(1)	53(1)	42(1)	13(1)	10(1)	24(1)
C(1')	43(1)	37(1)	60(1)	11(1)	17(1)	20(1)
C(2')	40(1)	30(1)	51(1)	9(1)	12(1)	17(1)
C(3')	48(1)	38(1)	44(1)	12(1)	14(1)	21(1)
C(4')	41(1)	40(1)	47(1)	5(1)	5(1)	17(1)
C(5')	40(1)	45(1)	55(1)	11(1)	14(1)	13(1)
C(6')	51(1)	40(1)	45(1)	12(1)	14(1)	17(1)
C(7')	44(1)	38(1)	46(1)	9(1)	6(1)	15(1)
C(8')	48(1)	93(2)	75(2)	0(1)	0(1)	35(1)
C(9')	76(2)	86(2)	45(1)	19(1)	11(1)	32(1)
C(10')	42(1)	42(1)	60(1)	14(1)	22(1)	18(1)
C(11')	39(1)	43(1)	54(1)	16(1)	23(1)	18(1)
C(12')	37(1)	43(1)	56(1)	15(1)	24(1)	17(1)
C(13')	46(1)	58(1)	66(1)	14(1)	17(1)	26(1)
C(14')	48(1)	66(2)	68(2)	3(1)	8(1)	22(1)
C(15')	63(1)	51(1)	74(2)	1(1)	18(1)	13(1)

C(16')	66(1)	44(1)	72(2)	14(1)	28(1)	21(1)
C(17')	46(1)	44(1)	60(1)	17(1)	28(1)	18(1)
C(18')	57(1)	49(1)	65(1)	26(1)	29(1)	29(1)
C(19')	50(1)	54(1)	53(1)	23(1)	26(1)	24(1)
C(20')	68(2)	76(2)	60(1)	30(1)	24(1)	39(1)
C(21')	71(2)	92(2)	56(1)	21(1)	9(1)	34(2)
C(22')	71(2)	71(2)	52(1)	7(1)	14(1)	20(1)
C(23')	64(1)	52(1)	53(1)	13(1)	21(1)	21(1)
C(24')	45(1)	48(1)	49(1)	17(1)	24(1)	18(1)
O(1)	114(2)	56(1)	85(1)	16(1)	−11(1)	52(1)
O(2)	83(1)	44(1)	48(1)	3(1)	0(1)	33(1)
P(1')	52(1)	56(1)	45(1)	4(1)	9(1)	30(1)
P(1)	56(1)	38(1)	106(1)	11(1)	30(1)	11(1)
F(1')	58(1)	97(1)	99(1)	23(1)	22(1)	27(1)
F(1)	243(3)	150(2)	179(3)	57(2)	142(2)	112(2)
F(2')	98(1)	76(1)	83(1)	−5(1)	13(1)	55(1)
F(2)	82(1)	72(1)	247(3)	8(2)	−18(2)	8(1)
F(3')	97(1)	94(1)	51(1)	13(1)	5(1)	48(1)
F(3)	98(1)	65(1)	168(2)	40(1)	34(1)	34(1)
Cl(1)	62(1)	54(1)	41(1)	1(1)	−6(1)	32(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for p.

	x	y	z	U(eq)
H(1'A)	1887	2037	3330	44
H(1'D)	1087	1729	2468	44
H(1A)	−1709	93	−645	45
H(1D)	−813	1145	−31	45
H(1B)	−282	1250	−1335	52
H(1C)	−656	2258	−1083	52
H(3A)	−2026	2519	−2189	55
H(5A)	−4442	−147	−4110	54
H(7A)	−2268	−702	−2178	51
H(8A)	−3564	3541	−3707	174
H(8B)	−2291	3500	−3342	174
H(8C)	−3251	3336	−2763	174
H(9A)	−5074	−3085	−4458	98
H(9B)	−4627	−1881	−4757	98
H(9C)	−5582	−2193	−4167	98
H(10A)	−3144	878	−848	47
H(10B)	−2190	1952	−134	47
H(13A)	−3820	−1016	−1122	63
H(14A)	−5259	−2912	−1464	82
H(15A)	−6311	−3795	−453	93
H(16A)	−5891	−2795	903	80
H(18A)	−4804	−933	1956	64
H(20A)	−3807	930	3003	74
H(21A)	−2430	2829	3387	83
H(22A)	−1258	3734	2435	76
H(23A)	−1494	2740	1106	62
H(1'B)	1402	3642	3606	54
H(1'C)	827	3367	2606	54
H(3'A)	3649	4343	4152	51
H(5'A)	5919	5450	2547	58
H(7'A)	2191	3822	1605	53
H(8'A)	7712	5806	4590	111
H(8'B)	7363	6112	3687	111
H(8'C)	7078	4820	3761	111
H(9'A)	3659	4348	−95	105
H(9'B)	2693	4392	434	105
H(9'C)	3056	3347	404	105
H(10C)	−675	1135	2921	56
H(10D)	71	1783	3870	56
H(13B)	−1611	−390	2074	66
H(14B)	−2735	−2169	1201	76
H(15B)	−2384	−3766	1503	80
H(16B)	−952	−3580	2696	72
H(18B)	579	−2397	4031	63

H(20B)	2150	−1251	5372	76
H(21B)	3322	485	6287	88
H(22B)	3090	2147	6007	83
H(23B)	1713	2062	4816	68

Crystal Data of the V-shaped compound **3** (R = OMe)

Table 1. Crystal data and structure refinement for p.

CCDC code	784762
Identification code	WY206
Empirical formula	$C_{21}H_{19}N_3O_2$
Formula weight	345.39
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, *A*ba2
Unit cell dimensions	a = 7.1660(6) Å α = 90 °
	b = 40.204(3) Å β = 90 °
	c = 6.3427(5) Å γ = 90 °
Volume	1827.4(3) Å^3
Z, Calculated density	4, 1.255 Mg/m^3
Absorption coefficient	0.083 mm^{-1}
F(000)	728
Crystal size	0.40 x 0.30 x 0.20 mm
Theta range for data collection	1.01 to 27.95 °
Limiting indices	$-7 \le h \le 9$, $-52 \le k \le 52$, $-8 \le l \le 6$
Reflections collected / unique	6680 / 2019 [R_{int} = 0.0504]
Completeness to θ = 27.95	99.5 %
Absorption correction	multi-scan
Max. and min. transmission	0.7456 and 0.6521
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2019 / 1 / 119
Goodness-of-fit on F^2	1.000
Final R indices [I > 2σ(I)]	R_1 = 0.0439, $_wR_2$ = 0.0920
R indices (all data)	R_1 = 0.0926, $_wR_2$ = 0.1147
Absolute structure parameter	1(2)
Largest diff. peak and hole	0.123 and −0.230 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for p.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	−94(2)	2110(1)	4471(3)	53(1)
C(1)	−30(4)	285(1)	154(4)	48(1)
C(2)	−43(4)	293(1)	−2011(5)	60(1)
C(3)	0	0	−3110(7)	70(1)
C(4)	−85(4)	593(1)	1405(5)	55(1)
C(5)	−68(3)	1173(1)	1698(4)	41(1)
C(6)	−872(3)	1449(1)	739(4)	44(1)
C(7)	−881(3)	1754(1)	1708(4)	42(1)
C(8)	−28(3)	1795(1)	3653(4)	41(1)
C(9)	821(3)	1526(1)	4624(4)	47(1)
C(10)	769(3)	1218(1)	3649(4)	47(1)
C(11)	842(5)	2173(1)	6407(5)	70(1)
N(1)	0	0	1255(5)	52(1)
N(2)	−84(3)	874(1)	531(4)	46(1)

Table 3. Bond lengths [Å] and angles [°] for p.

O(1)-C(8)	1.371(2)
O(1)-C(11)	1.422(3)
C(1)-N(1)	1.343(3)
C(1)-C(2)	1.374(4)
C(1)-C(4)	1.469(3)
C(2)-C(3)	1.369(3)
C(3)-C(2)#1	1.369(3)
C(4)-N(2)	1.258(3)
C(5)-C(10)	1.387(4)
C(5)-C(6)	1.391(3)
C(5)-N(2)	1.413(3)
C(6)-C(7)	1.371(3)
C(7)-C(8)	1.387(4)
C(8)-C(9)	1.383(3)
C(9)-C(10)	1.385(3)
N(1)-C(1)#1	1.343(3)
C(8)-O(1)-C(11)	118.31(18)
N(1)-C(1)-C(2)	122.6(2)
N(1)-C(1)-C(4)	116.0(2)
C(2)-C(1)-C(4)	121.4(2)
C(3)-C(2)-C(1)	119.3(3)
C(2)#1-C(3)-C(2)	118.8(4)
N(2)-C(4)-C(1)	121.2(2)
C(10)-C(5)-C(6)	117.7(2)
C(10)-C(5)-N(2)	125.6(2)
C(6)-C(5)-N(2)	116.6(2)
C(7)-C(6)-C(5)	121.3(2)
C(6)-C(7)-C(8)	120.1(2)
O(1)-C(8)-C(9)	124.7(2)
O(1)-C(8)-C(7)	115.5(2)
C(9)-C(8)-C(7)	119.9(2)
C(8)-C(9)-C(10)	119.2(2)
C(9)-C(10)-C(5)	121.8(2)
C(1)#1-N(1)-C(1)	117.3(3)
C(4)-N(2)-C(5)	122.3(2)

Symmetry transformations used to generate equivalent atoms: #1 −x, −y, z

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for p.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2$ [h^2 a^{*2} U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(1)	71(1)	36(1)	53(1)	−1(1)	−6(1)	4(1)
C(1)	67(2)	36(2)	41(2)	0(1)	1(1)	−2(1)
C(2)	97(2)	40(1)	44(2)	7(1)	−4(2)	0(1)
C(3)	123(4)	55(2)	33(2)	0	0	−1(2)
C(4)	82(2)	40(1)	42(2)	1(1)	5(2)	−4(1)
C(5)	47(1)	34(1)	41(2)	2(1)	−1(2)	−2(1)
C(6)	50(2)	43(1)	37(1)	4(1)	−5(1)	1(1)
C(7)	48(1)	34(1)	44(2)	8(1)	−3(2)	3(1)
C(8)	44(1)	32(1)	46(2)	3(1)	6(1)	1(1)
C(9)	56(1)	42(1)	42(1)	3(1)	−6(1)	0(1)
C(10)	55(2)	35(1)	51(2)	7(1)	−7(2)	3(1)
C(11)	98(2)	48(2)	63(2)	−14(2)	−16(2)	0(2)
N(1)	80(2)	36(2)	40(2)	0	0	−5(1)
N(2)	56(1)	37(1)	47(1)	−1(1)	−3(1)	−2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for p.

	x	y	z	U(eq)
H(2A)	−81	495	−2723	72
H(3)	0	0	−4577	84
H(4A)	−121	579	2868	66
H(6A)	−1415	1427	−585	52
H(7A)	−1460	1934	1059	51
H(9A)	1418	1553	5915	56
H(10A)	1310	1037	4322	56
H(11A)	669	2402	6801	104
H(11B)	2150	2128	6242	104
H(11C)	339	2032	7486	104

Crystal Data of the V-shaped compound **5** (R = Me)

Table 1. Crystal data and structure refinement for p.

CCDC code	784763
Identification code	wy201
Empirical formula	$C_{21}H_{19}N_3$
Formula weight	313.39
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, *P*2/*c*
Unit cell dimensions	a = 4.7249(7) Å α = 90 °
	b = 6.2811(9) Å β = 94.639(3) °
	c = 28.965(4) Å γ = 90 °
Volume	856.8(2) Å^3
Z, Calculated density	2, 1.215 Mg/m^3
Absorption coefficient	0.073 mm^{-1}
F(000)	332
Crystal size	0.50 x 0.40 x 0.30 mm
Theta range for data collection	1.41 to 25.25 °
Limiting indices	$-5 \le h \le 5$, $-7 \le k \le 7$, $-34 \le l \le 34$
Reflections collected / unique	11557 / 1566 [R_{int} = 0.0405]
Completeness to θ = 25.25	99.7 %
Absorption correction	multi-scan
Max. and min. transmission	0.7456 and 0.5906
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1566 / 0 / 111
Goodness-of-fit on F^2	3.356
Final *R* indices [I > 2σ(I)]	R_1 = 0.1742, $_wR_2$ = 0.6124
R indices (all data)	R_1 = 0.1810, $_wR_2$ = 0.6184
Extinction coefficient	0.31(18)
Largest diff. peak and hole	0.544 and −0.451 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for p.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	0	6305(10)	2500	48(2)
N(2)	5501(10)	6935(8)	3400(2)	53(2)
C(1)	0	10724(13)	2500	60(3)
C(2)	1842(12)	9622(10)	2801(2)	56(2)
C(3)	1797(11)	7400(9)	2795(2)	45(2)
C(4)	3709(12)	6109(9)	3107(2)	50(2)
C(5)	7361(12)	5638(9)	3683(2)	48(2)
C(6)	8606(15)	6494(11)	4085(2)	63(2)
C(7)	10497(14)	5365(12)	4369(2)	68(2)
C(8)	11291(13)	3287(12)	4268(2)	61(2)
C(9)	10077(14)	2446(11)	3848(2)	64(2)
C(10)	8197(14)	3556(10)	3563(2)	59(2)
C(11)	13379(17)	2040(15)	4572(3)	86(3)

Table 3. Bond lengths [Å] and angles [°] for p.

N(1)-C(3)	1.344(6)
N(1)-C(3)#1	1.344(6)
N(2)-C(4)	1.260(6)
N(2)-C(5)	1.411(7)
C(1)-C(2)	1.369(7)
C(1)-C(2)#1	1.369(7)
C(2)-C(3)	1.396(9)
C(3)-C(4)	1.470(7)
C(5)-C(6)	1.372(8)
C(5)-C(10)	1.417(9)
C(6)-C(7)	1.363(8)
C(7)-C(8)	1.396(11)
C(8)-C(9)	1.404(9)
C(8)-C(11)	1.491(8)
C(9)-C(10)	1.356(8)
C(3)-N(1)-C(3)#1	118.4(6)
C(4)-N(2)-C(5)	120.4(5)
C(2)-C(1)-C(2)#1	119.3(7)
C(1)-C(2)-C(3)	119.2(5)
N(1)-C(3)-C(2)	121.9(5)
N(1)-C(3)-C(4)	115.7(5)
C(2)-C(3)-C(4)	122.3(5)
N(2)-C(4)-C(3)	122.2(5)
C(6)-C(5)-N(2)	118.1(5)
C(6)-C(5)-C(10)	117.4(5)
N(2)-C(5)-C(10)	124.3(5)
C(7)-C(6)-C(5)	121.5(6)
C(6)-C(7)-C(8)	122.3(6)
C(7)-C(8)-C(9)	115.8(6)
C(7)-C(8)-C(11)	122.9(6)
C(9)-C(8)-C(11)	121.3(7)
C(10)-C(9)-C(8)	122.4(6)
C(9)-C(10)-C(5)	120.5(6)

Symmetry transformations used to generate equivalent atoms: #1 −x, y, −z+1/2

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for p.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2$ [h^2 a^{*2} U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(1)	49(4)	39(3)	52(4)	0	−12(3)	0
N(2)	61(3)	48(3)	49(3)	−3(2)	−6(2)	−4(2)
C(1)	70(6)	38(4)	71(6)	0	−3(4)	0
C(2)	64(4)	46(4)	57(4)	−5(2)	2(3)	−4(2)
C(3)	52(4)	41(3)	43(3)	−2(2)	3(2)	−10(2)
C(4)	53(4)	44(3)	51(4)	4(2)	−7(3)	−9(2)
C(5)	47(3)	49(3)	48(3)	4(2)	−1(2)	−4(2)
C(6)	75(4)	56(4)	55(4)	2(3)	−4(3)	1(3)
C(7)	65(4)	80(5)	54(4)	1(3)	−17(3)	−4(3)
C(8)	49(4)	74(4)	59(4)	14(3)	−2(3)	−1(3)
C(9)	65(4)	59(4)	67(4)	5(3)	−1(3)	7(3)
C(10)	62(4)	62(4)	51(3)	−7(3)	−6(3)	−1(3)
C(11)	86(5)	98(6)	71(5)	23(4)	−12(4)	24(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for p.

	x	y	z	U(eq)
H(1)	0	12205	2500	72
H(2B)	3109	10346	3008	67
H(4A)	3592	4633	3088	60
H(6A)	8150	7878	4166	75
H(7A)	11286	6001	4639	81
H(9A)	10580	1079	3763	77
H(10A)	7450	2947	3287	71
H(11A)	13978	2867	4841	129
H(11B)	14996	1703	4405	129
H(11C)	12506	747	4666	129

Crystal Data of the V-shaped compound **8** (R = F)

Table 1. Crystal data and structure refinement for p.

CCDC code	798464
Identification code	wy209
Empirical formula	$C_{19}H_{13}F_2N_3$
Formula weight	321.32
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	a = 35.041(6) Å alpha = 90 ° b = 6.2652(11) Å beta = 92.850(3) ° c = 7.1363(12) Å gamma = 90 °
Volume	1564.7(5) A^3
Z, Calculated density	4, 1.364 Mg/m^3
Absorption coefficient	0.099 mm^{-1}
F(000)	664
Crystal size	0.50 x 0.40 x 0.30 mm
Theta range for data collection	3.30 to 25.24 °
Limiting indices	-41<=h<=42, -3<=k<=7, -8<=l<=6
Reflections collected / unique	5197 / 1407 [R(int) = 0.0395]
Completeness to theta = 25.24	98.5 %
Absorption correction	multi-scan
Max. and min. transmission	0.7457 and 0.6233
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1407 / 0 / 110
Goodness-of-fit on F^2	1.054
Final R indices [I>2sigma(I)]	R1 = 0.0471, wR2 = 0.1245
R indices (all data)	R1 = 0.0607, wR2 = 0.1442
Largest diff. peak and hole	0.216 and -0.200 $Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for p.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
F(1)	2232(1)	5066(3)	638(2)	88(1)
N(1)	0	454(3)	2500	41(1)
C(4)	664(1)	652(3)	1960(3)	44(1)
C(1)	320(1)	-655(3)	2210(2)	39(1)
C(2)	330(1)	-2877(3)	2179(3)	49(1)
C(3)	0	-3993(4)	2500	55(1)
N(2)	978(1)	-131(2)	1490(2)	43(1)
C(5)	1293(1)	1252(3)	1259(2)	40(1)
C(6)	1655(1)	507(3)	1777(3)	48(1)
C(7)	1972(1)	1792(4)	1593(3)	58(1)
C(8)	1920(1)	3802(4)	826(3)	56(1)
C(9)	1569(1)	4573(3)	257(3)	52(1)
C(10)	1254(1)	3296(3)	465(3)	45(1)

Table 3. Bond lengths [Å] and angles [°] for p.

F(1)-C(8)	1.363(2)
N(1)-C(1)	1.3453(19)
N(1)-C(1)#1	1.3454(19)
C(4)-N(2)	1.264(2)
C(4)-C(1)	1.473(2)
C(1)-C(2)	1.393(3)
C(2)-C(3)	1.379(2)
C(3)-C(2)#1	1.379(2)
N(2)-C(5)	1.419(2)
C(5)-C(6)	1.386(2)
C(5)-C(10)	1.404(3)
C(6)-C(7)	1.384(3)
C(7)-C(8)	1.381(3)
C(8)-C(9)	1.365(3)
C(9)-C(10)	1.377(3)
C(1)-N(1)-C(1)#1	117.8(2)
N(2)-C(4)-C(1)	122.87(17)
N(1)-C(1)-C(2)	122.61(17)
N(1)-C(1)-C(4)	115.13(16)
C(2)-C(1)-C(4)	122.26(16)
C(3)-C(2)-C(1)	118.96(18)
C(2)-C(3)-C(2)#1	119.0(2)
C(4)-N(2)-C(5)	119.05(15)
C(6)-C(5)-C(10)	118.91(17)
C(6)-C(5)-N(2)	118.09(16)
C(10)-C(5)-N(2)	122.95(15)
C(7)-C(6)-C(5)	120.54(19)
C(8)-C(7)-C(6)	118.47(18)
F(1)-C(8)-C(9)	118.8(2)
F(1)-C(8)-C(7)	118.51(19)
C(9)-C(8)-C(7)	122.71(18)
C(8)-C(9)-C(10)	118.53(19)
C(9)-C(10)-C(5)	120.78(17)

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1/2

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for p.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2$ [h^2 a^{*2} U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
F(1)	62(1)	102(1)	99(1)	7(1)	5(1)	-36(1)
N(1)	41(1)	32(1)	48(1)	0	4(1)	0
C(4)	45(1)	34(1)	52(1)	-1(1)	3(1)	0(1)
C(1)	41(1)	34(1)	42(1)	-1(1)	1(1)	2(1)
C(2)	46(1)	34(1)	67(1)	-2(1)	1(1)	6(1)
C(3)	57(2)	29(1)	79(2)	0	0(1)	0
N(2)	41(1)	40(1)	47(1)	0(1)	2(1)	2(1)
C(5)	41(1)	42(1)	39(1)	-4(1)	4(1)	0(1)
C(6)	44(1)	51(1)	51(1)	1(1)	3(1)	7(1)
C(7)	39(1)	78(2)	57(1)	-2(1)	0(1)	4(1)
C(8)	47(1)	70(2)	53(1)	-4(1)	6(1)	-17(1)
C(9)	60(1)	50(1)	48(1)	2(1)	6(1)	-8(1)
C(10)	42(1)	47(1)	47(1)	1(1)	2(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for p.

	x	y	z	U(eq)
H(4A)	649	2116	2157	52
H(2B)	554	-3596	1945	58
H(3)	0	-5478	2500	66
H(6A)	1685	-868	2253	58
H(7A)	2215	1314	1976	70
H(9A)	1543	5932	-259	63
H(10A)	1013	3793	75	54