Figure S1: ^{1}H NMR spectrum of **1** in $CDCl_3$

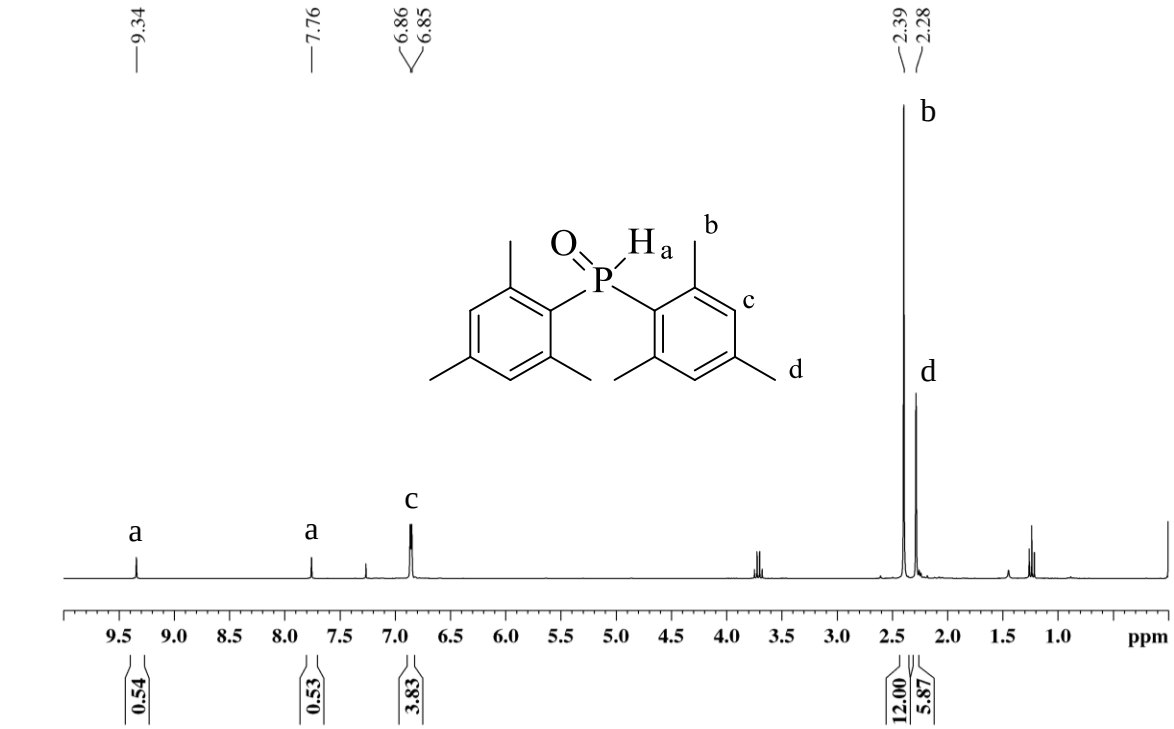


Figure S2: $^{1}H\{^{31}P\}$ NMR spectrum of **1** in $CDCl_3$

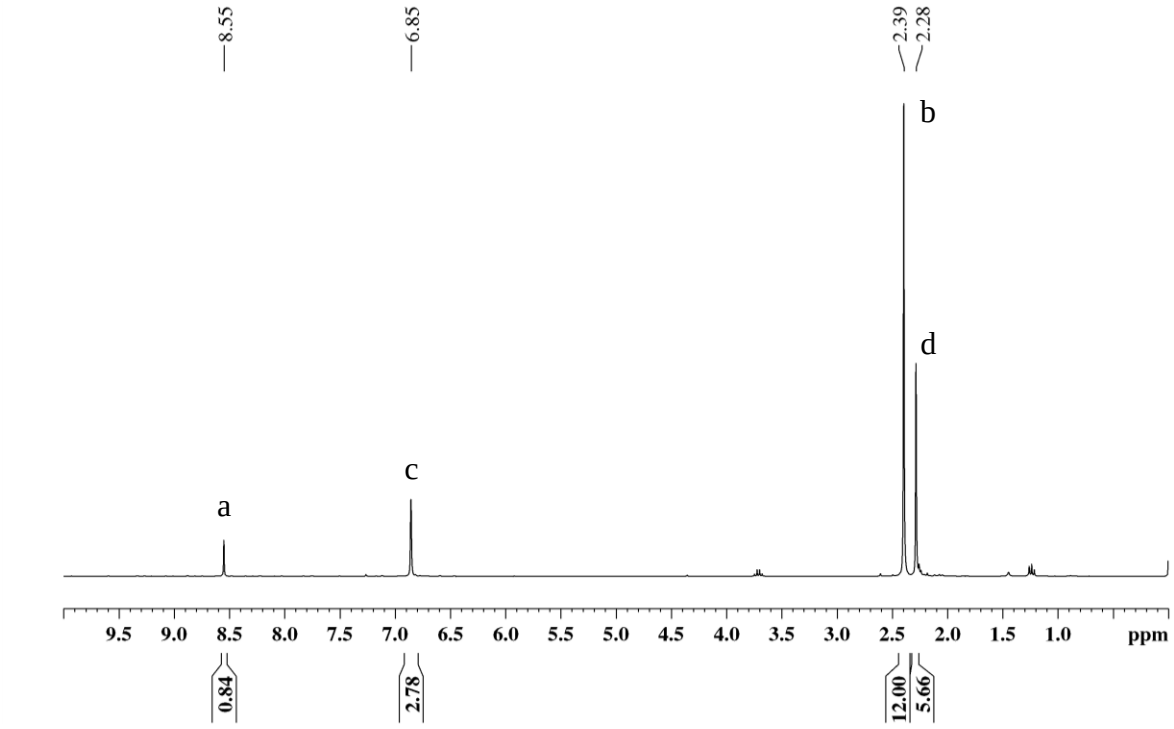


Figure S3: $^{13}C\{^{1}H\}$ NMR spectrum of **1** in $CDCl_3$

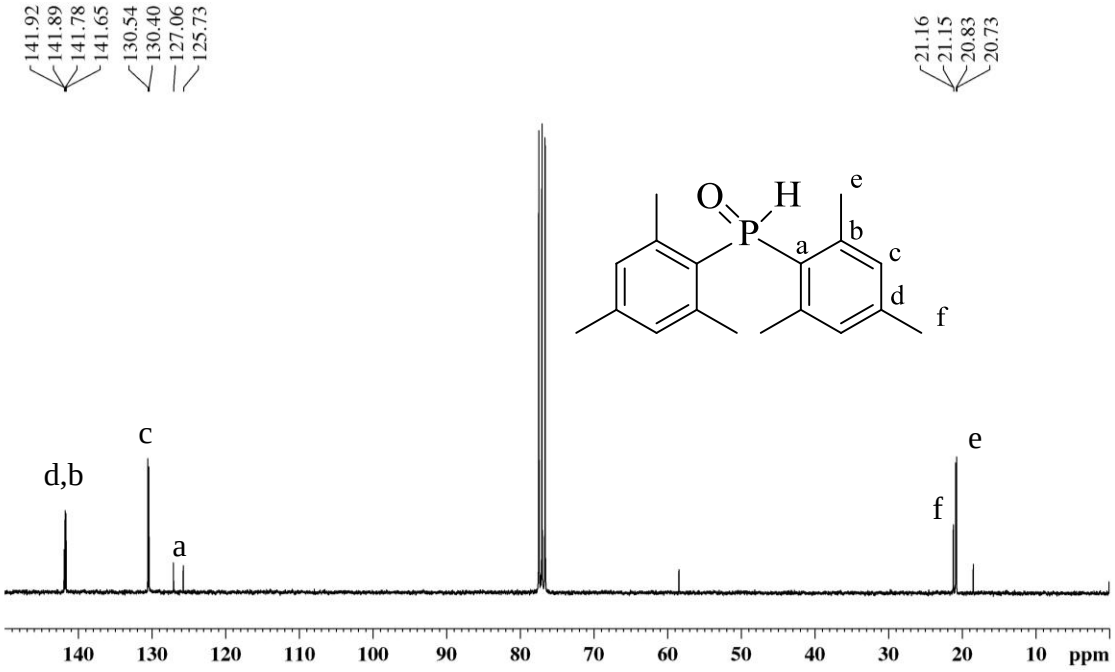


Figure S4: $^{31}P\{^{1}H\}$ NMR spectrum of **1** in $CDCl_3$

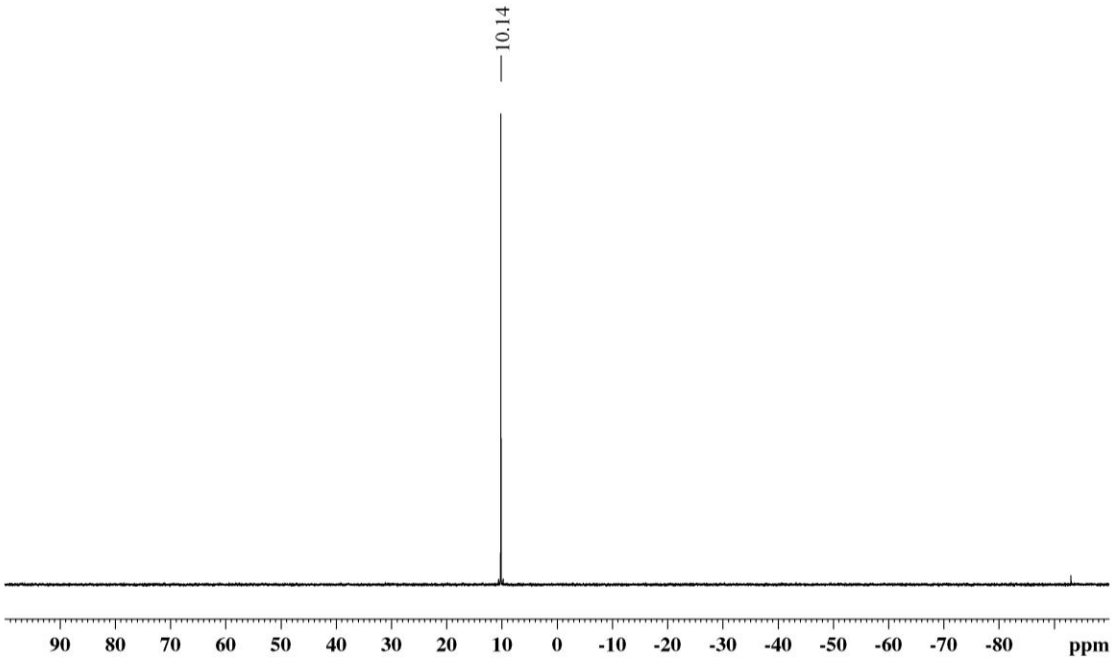


Figure S5: ^{31}P NMR spectrum of **1** in $CDCl_3$

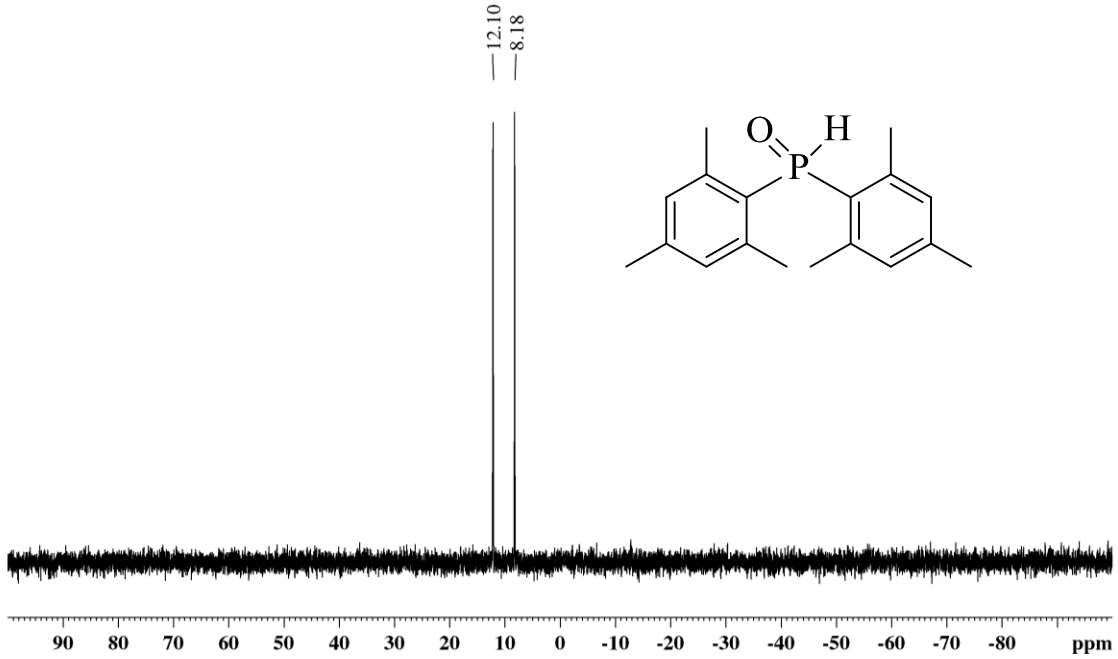
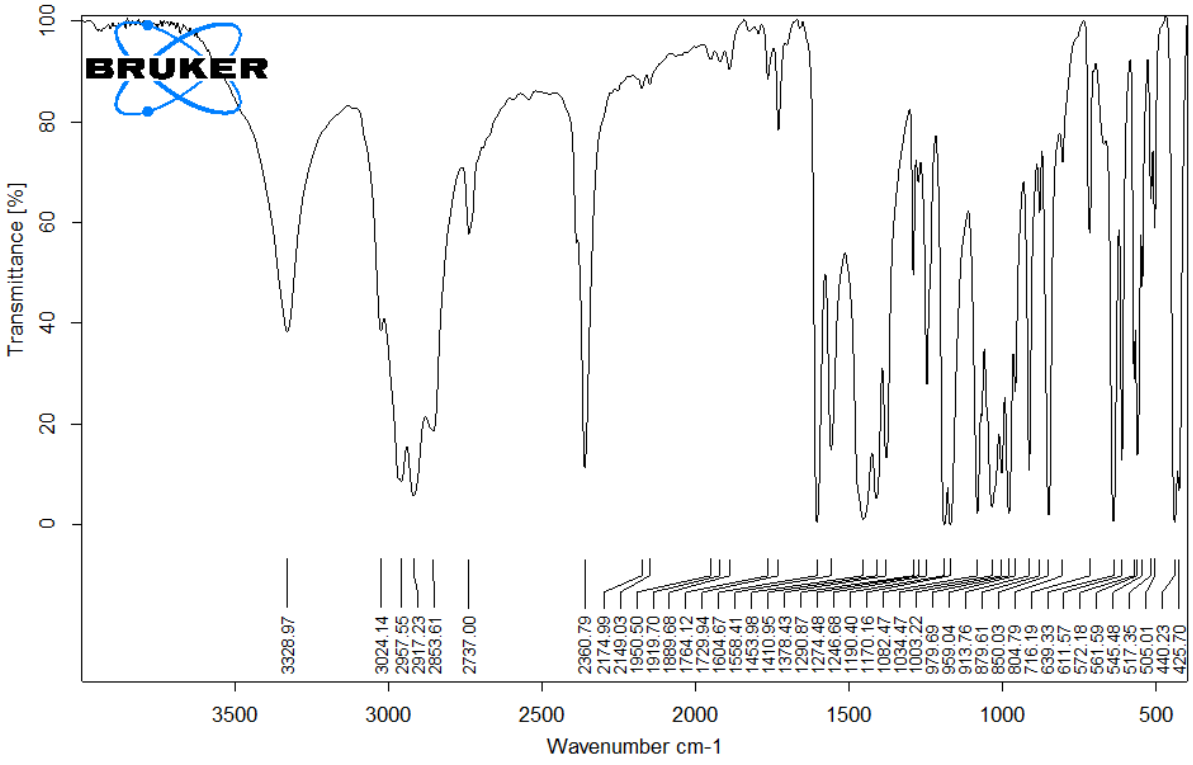


Figure S6: IR spectrum of **1** in (KBr pellet)



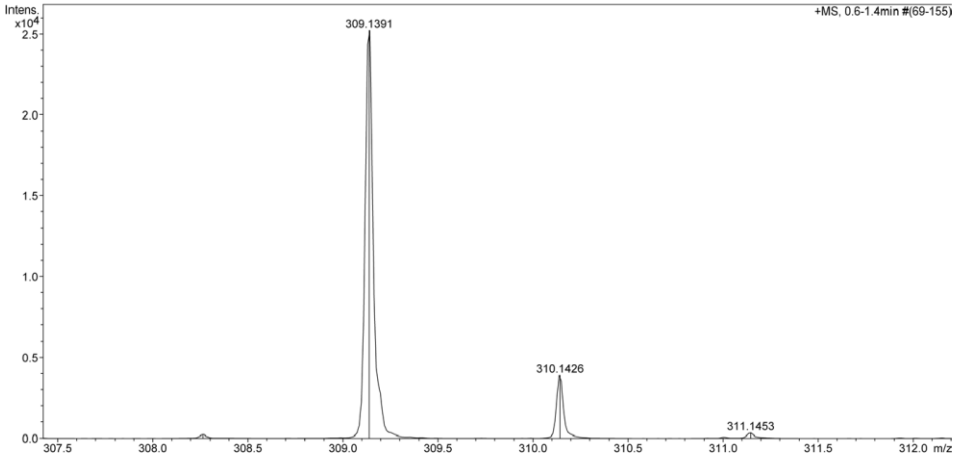
Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name	D:\Data\Xiao\July 13 2017000001.d	Acquisition Date	7/13/2017 10:25:15 AM
Method	Fengcurrent.m	Operator	Administrator
Sample Name	MeS2 POH	Instrument	micrOTOF 57
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Corrector Fill	45 V
Scan Range	n/a	Capillary Exit	100.0 V	Set Pulsar Pull	400 V
Scan Begin	50 m/z	Hexapole RF	140.0 V	Set Pulsar Push	400 V
Scan End	1500 m/z	Skimmer 1	50.0 V	Set Reflector	1300 V
		Hexapole 1	23.0 V	Set Flight Tube	9000 V
				Set Detector TOF	2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e⁻
C 18 H 23 Na 1 O 1 P 1	0.03	309.1379	-4.03	-3.97	7.50	ok	even

Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	5137(1)	3815(1)	7453(1)	18(1)
O(1)	7070(2)	3666(2)	7637(1)	26(1)
C(1)	3691(2)	2695(2)	6074(2)	17(1)
C(2)	2770(2)	3507(2)	5177(2)	19(1)
C(3)	1646(2)	2581(2)	4150(2)	22(1)
C(4)	1401(2)	884(2)	3973(2)	21(1)
C(5)	2368(2)	104(2)	4851(2)	22(1)
C(6)	3511(2)	966(2)	5890(2)	18(1)
C(7)	2939(3)	5351(2)	5257(2)	25(1)
C(8)	157(3)	-107(3)	2866(2)	30(1)
C(9)	4549(3)	10(2)	6780(2)	24(1)
C(10)	4296(2)	3321(2)	8572(2)	16(1)
C(11)	2559(2)	3743(2)	8541(2)	18(1)
C(12)	1890(2)	3388(2)	9390(2)	18(1)
C(13)	2852(2)	2620(2)	10270(2)	18(1)
C(14)	4556(2)	2230(2)	10298(2)	18(1)
C(15)	5316(2)	2574(2)	9477(2)	17(1)
C(16)	1389(2)	4600(2)	7636(2)	23(1)
C(17)	2066(3)	2244(2)	11169(2)	23(1)
C(18)	7219(2)	2152(2)	9645(2)	22(1)

Table S2. Bond lengths [Å] and angles [°] for **1**.

P(1)-O(1)	1.4854(13)
P(1)-C(1)	1.8151(18)
P(1)-C(10)	1.8162(18)
P(1)-H(1)	1.319(17)
C(1)-C(2)	1.411(2)
C(1)-C(6)	1.412(2)
C(2)-C(3)	1.392(3)
C(2)-C(7)	1.517(2)
C(3)-C(4)	1.388(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.389(3)
C(4)-C(8)	1.507(3)
C(5)-C(6)	1.388(3)
C(5)-H(5)	0.9500
C(6)-C(9)	1.509(2)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(15)	1.409(2)
C(10)-C(11)	1.417(2)
C(11)-C(12)	1.388(2)
C(11)-C(16)	1.507(2)
C(12)-C(13)	1.383(2)
C(12)-H(12)	0.9500
C(13)-C(14)	1.386(2)
C(13)-C(17)	1.506(2)
C(14)-C(15)	1.398(2)
C(14)-H(14)	0.9500

C(15)-C(18)	1.511(2)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800

O(1)-P(1)-C(1)	113.94(8)
O(1)-P(1)-C(10)	116.64(8)
C(1)-P(1)-C(10)	108.07(8)
O(1)-P(1)-H(1)	111.7(7)
C(1)-P(1)-H(1)	103.9(7)
C(10)-P(1)-H(1)	101.2(7)
C(2)-C(1)-C(6)	119.32(16)
C(2)-C(1)-P(1)	121.68(13)
C(6)-C(1)-P(1)	118.99(13)
C(3)-C(2)-C(1)	118.91(17)
C(3)-C(2)-C(7)	117.28(16)
C(1)-C(2)-C(7)	123.81(17)
C(4)-C(3)-C(2)	122.42(17)
C(4)-C(3)-H(3)	118.8
C(2)-C(3)-H(3)	118.8
C(3)-C(4)-C(5)	117.76(17)
C(3)-C(4)-C(8)	122.06(17)
C(5)-C(4)-C(8)	120.17(17)
C(6)-C(5)-C(4)	122.23(17)
C(6)-C(5)-H(5)	118.9
C(4)-C(5)-H(5)	118.9
C(5)-C(6)-C(1)	119.27(17)
C(5)-C(6)-C(9)	118.46(16)
C(1)-C(6)-C(9)	122.26(16)
C(2)-C(7)-H(7A)	109.5

C(2)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(2)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(4)-C(8)-H(8A)	109.5
C(4)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(4)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(6)-C(9)-H(9A)	109.5
C(6)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(6)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(15)-C(10)-C(11)	119.13(15)
C(15)-C(10)-P(1)	122.65(13)
C(11)-C(10)-P(1)	118.20(13)
C(12)-C(11)-C(10)	119.34(16)
C(12)-C(11)-C(16)	117.40(15)
C(10)-C(11)-C(16)	123.25(16)
C(13)-C(12)-C(11)	122.46(16)
C(13)-C(12)-H(12)	118.8
C(11)-C(12)-H(12)	118.8
C(12)-C(13)-C(14)	117.64(16)
C(12)-C(13)-C(17)	120.70(16)
C(14)-C(13)-C(17)	121.66(16)
C(13)-C(14)-C(15)	122.67(16)
C(13)-C(14)-H(14)	118.7
C(15)-C(14)-H(14)	118.7
C(14)-C(15)-C(10)	118.74(16)
C(14)-C(15)-C(18)	116.97(16)
C(10)-C(15)-C(18)	124.27(16)
C(11)-C(16)-H(16A)	109.5

C(11)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(11)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(13)-C(17)-H(17A)	109.5
C(13)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(13)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(15)-C(18)-H(18A)	109.5
C(15)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(15)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S3. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **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)	18(1)	19(1)	3(1)	7(1)	0(1)
O(1)	18(1)	32(1)	28(1)	4(1)	10(1)	0(1)
C(1)	17(1)	18(1)	18(1)	4(1)	10(1)	3(1)
C(2)	20(1)	20(1)	21(1)	6(1)	11(1)	4(1)
C(3)	21(1)	28(1)	19(1)	10(1)	8(1)	6(1)
C(4)	20(1)	26(1)	18(1)	1(1)	9(1)	-2(1)
C(5)	26(1)	18(1)	23(1)	3(1)	10(1)	0(1)
C(6)	20(1)	18(1)	20(1)	4(1)	9(1)	3(1)
C(7)	34(1)	20(1)	26(1)	9(1)	12(1)	7(1)
C(8)	26(1)	39(1)	21(1)	4(1)	6(1)	-5(1)
C(9)	30(1)	20(1)	23(1)	4(1)	7(1)	4(1)
C(10)	16(1)	15(1)	16(1)	0(1)	6(1)	0(1)
C(11)	18(1)	16(1)	17(1)	2(1)	4(1)	0(1)
C(12)	16(1)	18(1)	21(1)	3(1)	7(1)	2(1)
C(13)	18(1)	16(1)	19(1)	2(1)	7(1)	0(1)
C(14)	19(1)	18(1)	17(1)	4(1)	2(1)	2(1)
C(15)	15(1)	16(1)	19(1)	0(1)	4(1)	1(1)
C(16)	20(1)	27(1)	24(1)	10(1)	9(1)	7(1)
C(17)	23(1)	24(1)	25(1)	9(1)	10(1)	4(1)
C(18)	17(1)	27(1)	21(1)	6(1)	6(1)	5(1)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **1**.

	x	y	z	U(eq)
H(3)	1023	3130	3548	26
H(5)	2242	-1059	4736	27
H(7A)	2525	5611	4479	38
H(7B)	4191	5768	5636	38
H(7C)	2210	5865	5706	38
H(8A)	-329	622	2318	44
H(8B)	-823	-660	3025	44
H(8C)	814	-927	2535	44
H(9A)	4467	-1148	6424	36
H(9B)	4051	114	7416	36
H(9C)	5803	444	7077	36
H(12)	727	3682	9365	22
H(14)	5236	1707	10899	22
H(16A)	1269	3982	6868	34
H(16B)	1931	5708	7722	34
H(16C)	208	4669	7731	34
H(17A)	1064	1407	10809	34
H(17B)	1643	3244	11506	34
H(17C)	2982	1838	11776	34
H(18A)	7318	1602	8908	32
H(18B)	7552	1423	10209	32
H(18C)	8019	3159	9927	32
H(1)	4720(20)	5340(20)	7440(14)	9(4)