

## Synthesis and Solid-State Structures of Gold(I) Complexes of Diphosphines

Sebastian Molitor, Christoph Mahler and Viktoria H. Gessner<sup>\*</sup>

Institut für Anorganische Chemie, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074  
Würzburg, Germany

### Index

1. NMR spectra	S1
2. Crystal Structure Determination	S15
2.1 Crystal Structure Determination of <b>1d</b>	S18
2.2 Crystal Structure Determination of <b>1f</b>	S19
2.3 Crystal Structure Determination of <b>2a</b>	S21
2.4 Crystal Structure Determination of <b>2b</b>	S24
2.5 Crystal Structure Determination of <b>2c</b>	S26
2.6 Crystal Structure Determination of <b>2d</b>	S28
2.7 Crystal Structure Determination of <b>2e</b>	S30
2.8 Crystal Structure Determination of <b>2h</b>	S35
3. References	S37

## 1. $^1\text{H}$ NMR, $^{13}\text{C}\{^1\text{H}\}$ NMR, $^{13}\text{C}\{^1\text{H}\}$ DEPT135 NMR and $^{31}\text{P}\{^1\text{H}\}$ NMR spectra

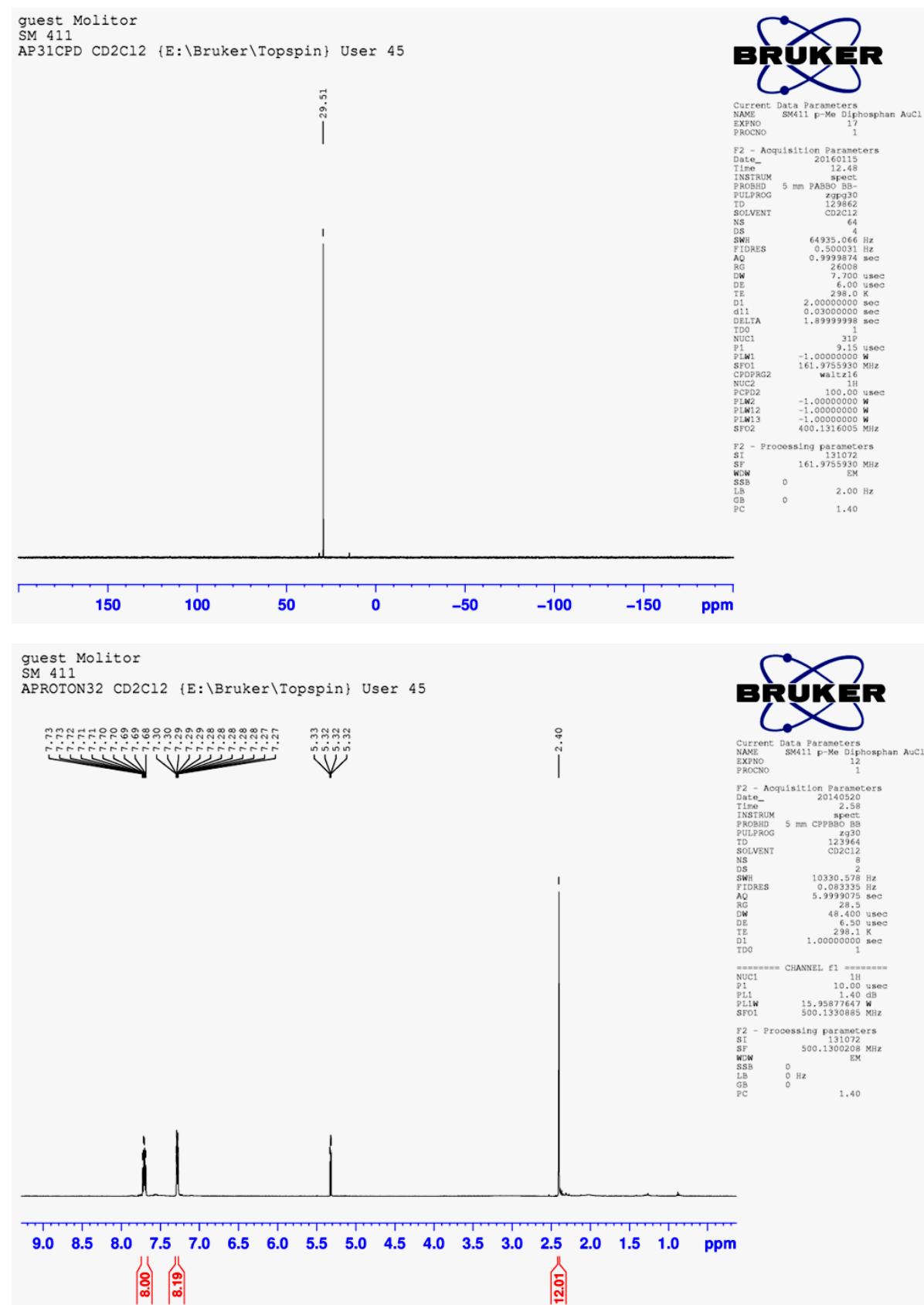


Figure S1a.  $^{31}\text{P}\{^1\text{H}\}$  NMR and  $^1\text{H}$  NMR spectra of **2a**.

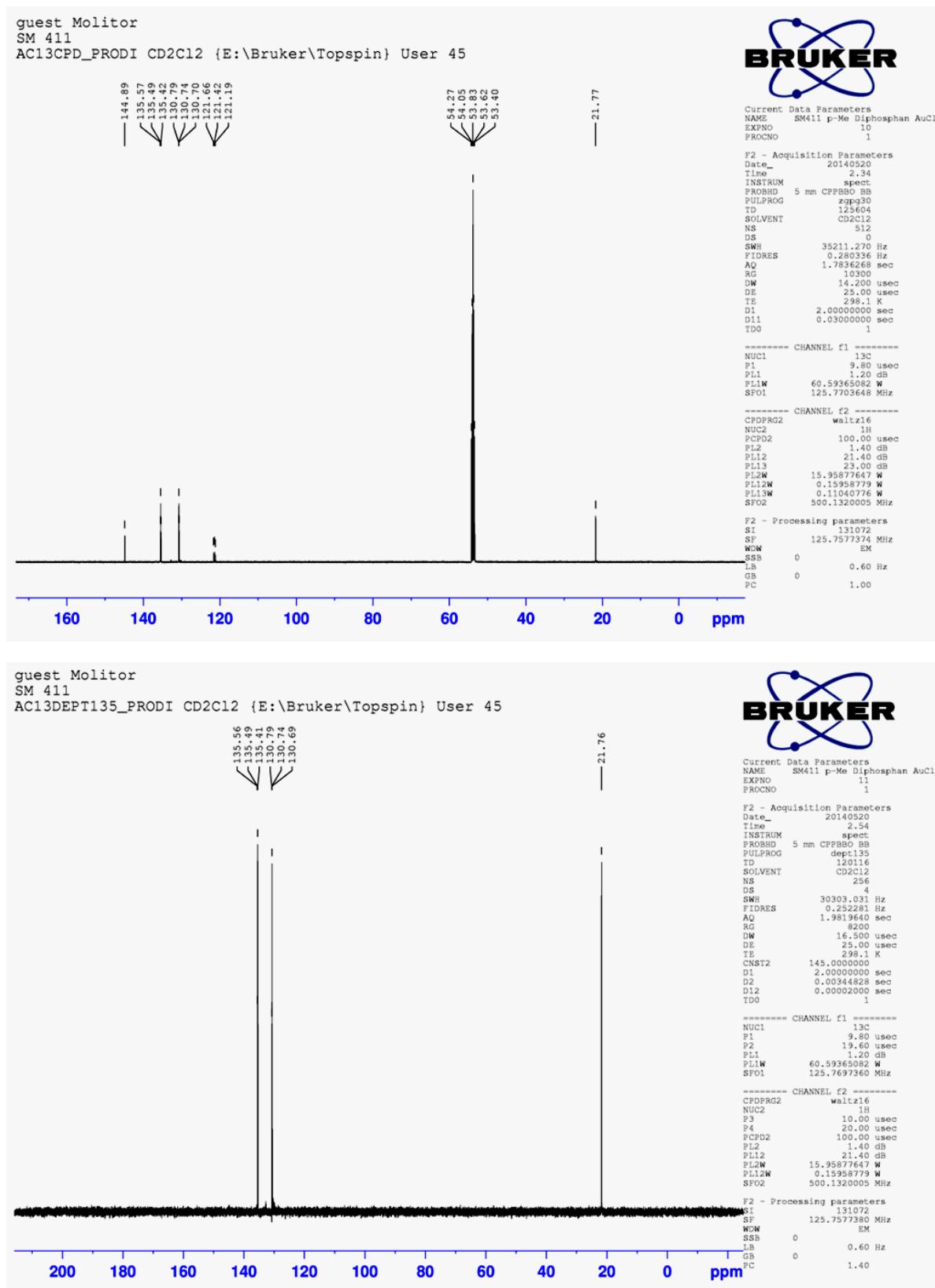
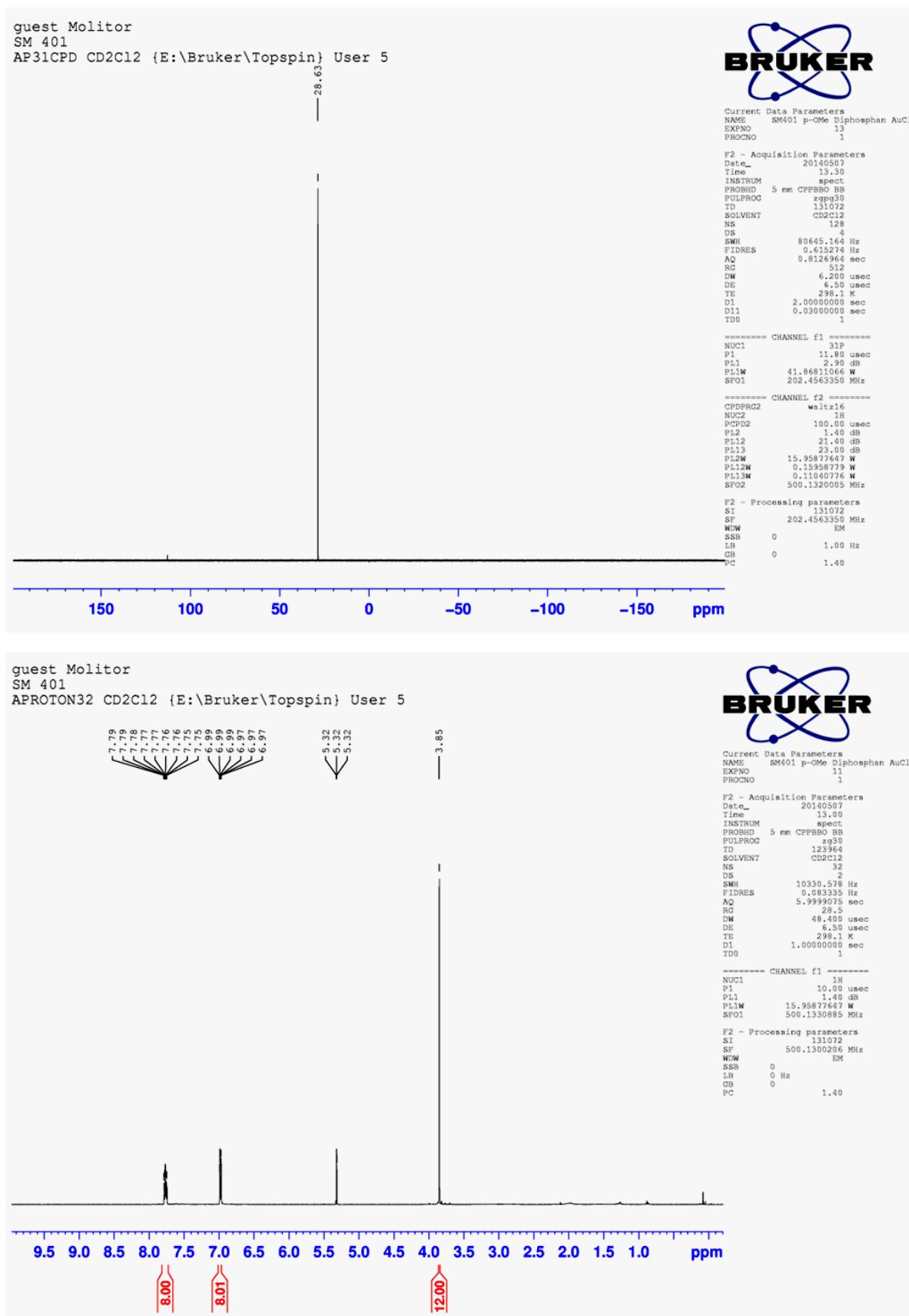


Figure S1b.  $^{13}\text{C}\{^1\text{H}\}$  NMR and  $^{13}\text{C}\{^1\text{H}\}$  DEPT135 NMR spectra of **2a**.

**Figure S2a.**  $^{31}\text{P}\{\text{H}\}$  NMR and  $^1\text{H}$  NMR spectra of **2b**.

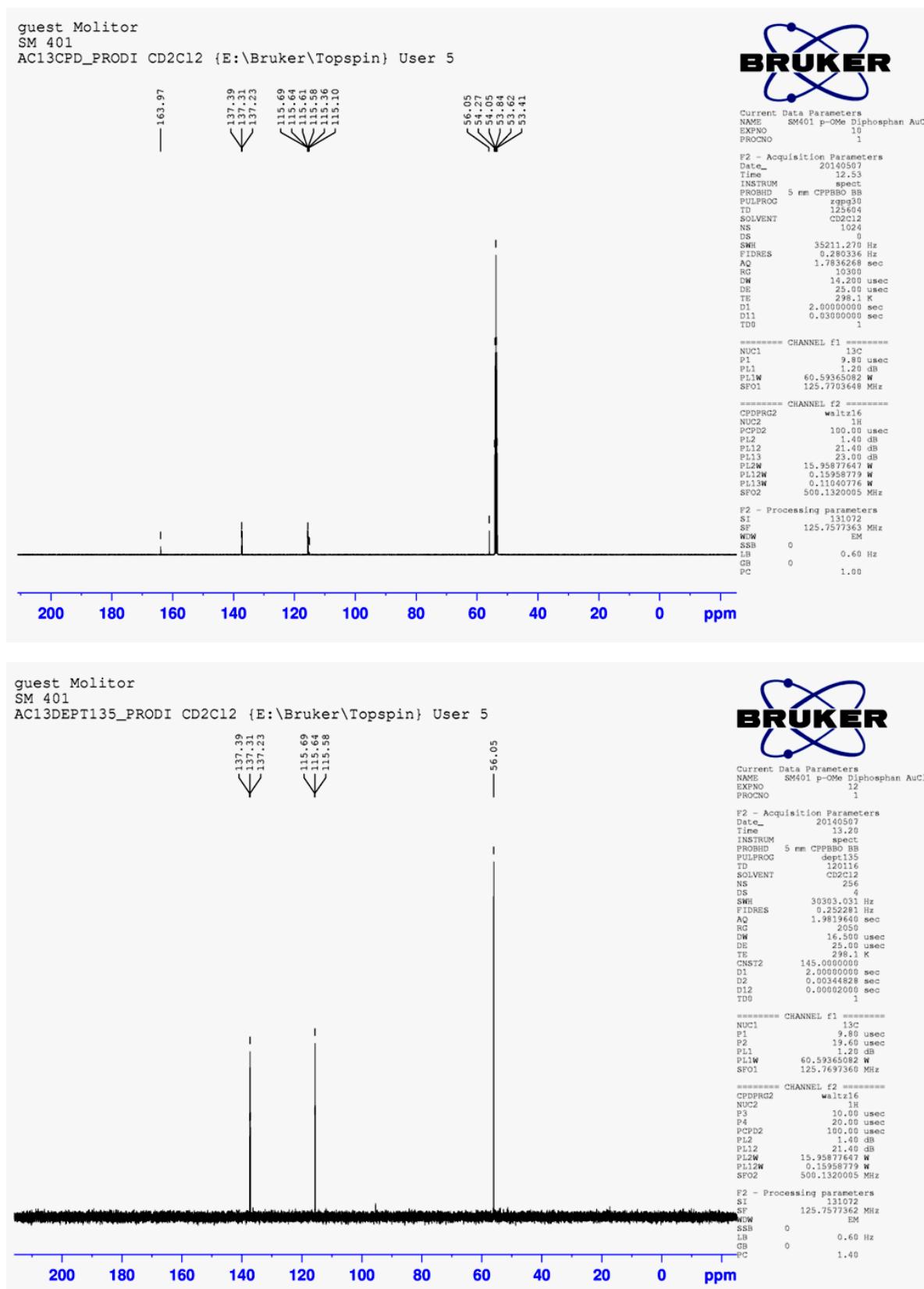


Figure S2b.  $^{13}\text{C}\{^1\text{H}\}$  NMR and  $^{13}\text{C}\{^1\text{H}\}$  DEPT135 NMR spectra of **2b**.

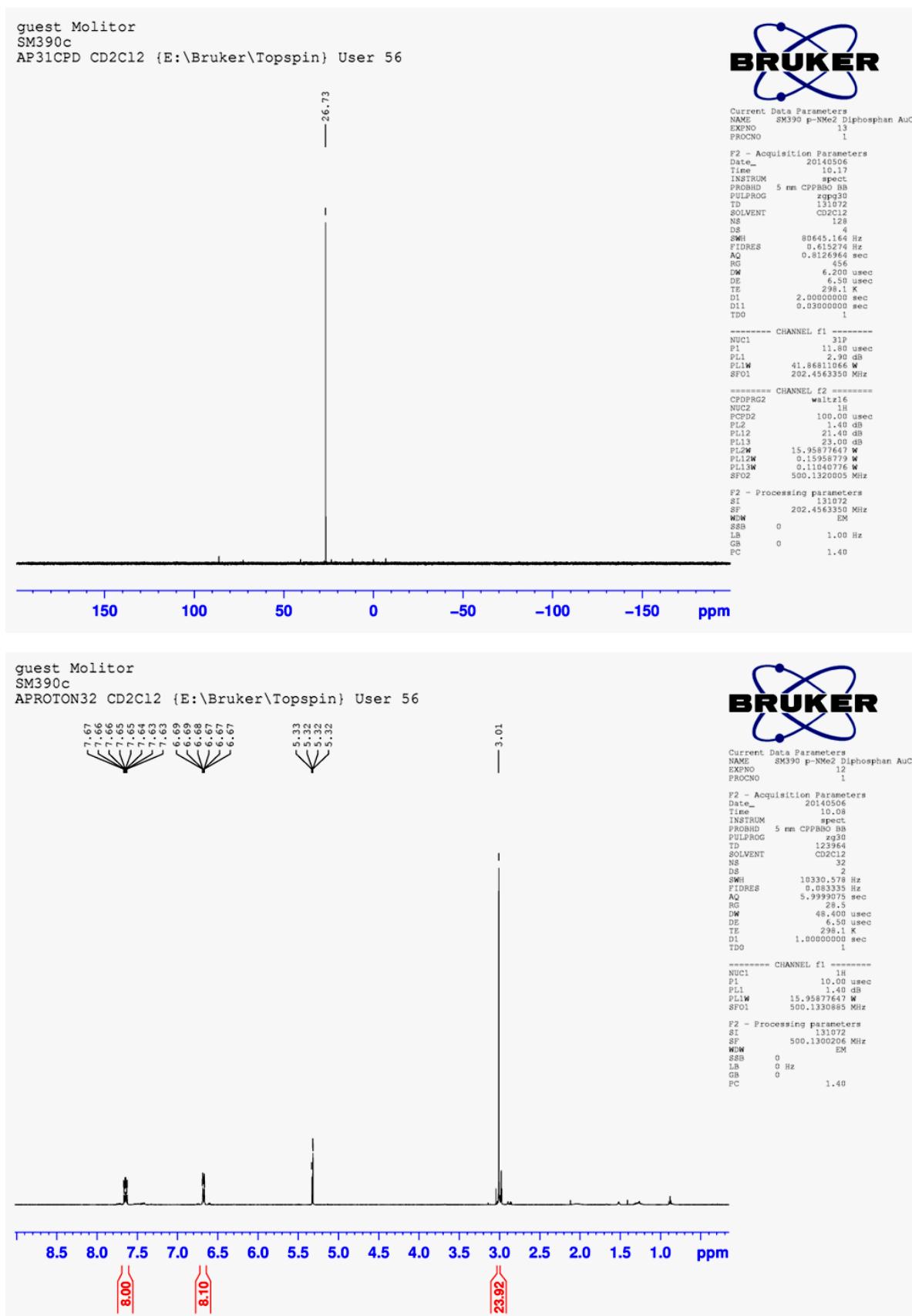


Figure S3a.  $^{31}\text{P}\{\text{H}\}$  NMR and  $^1\text{H}$  NMR spectra of **2c**.

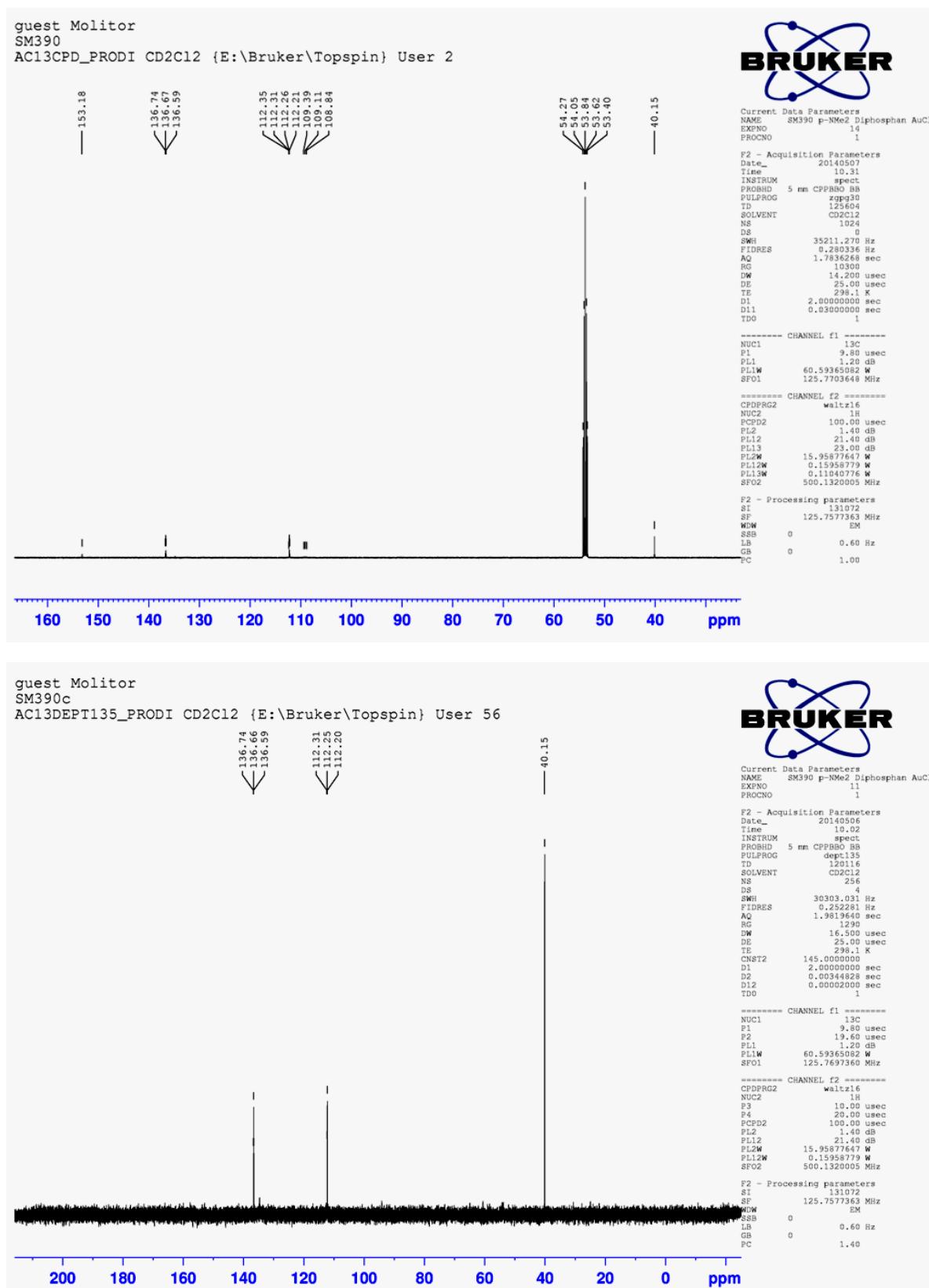
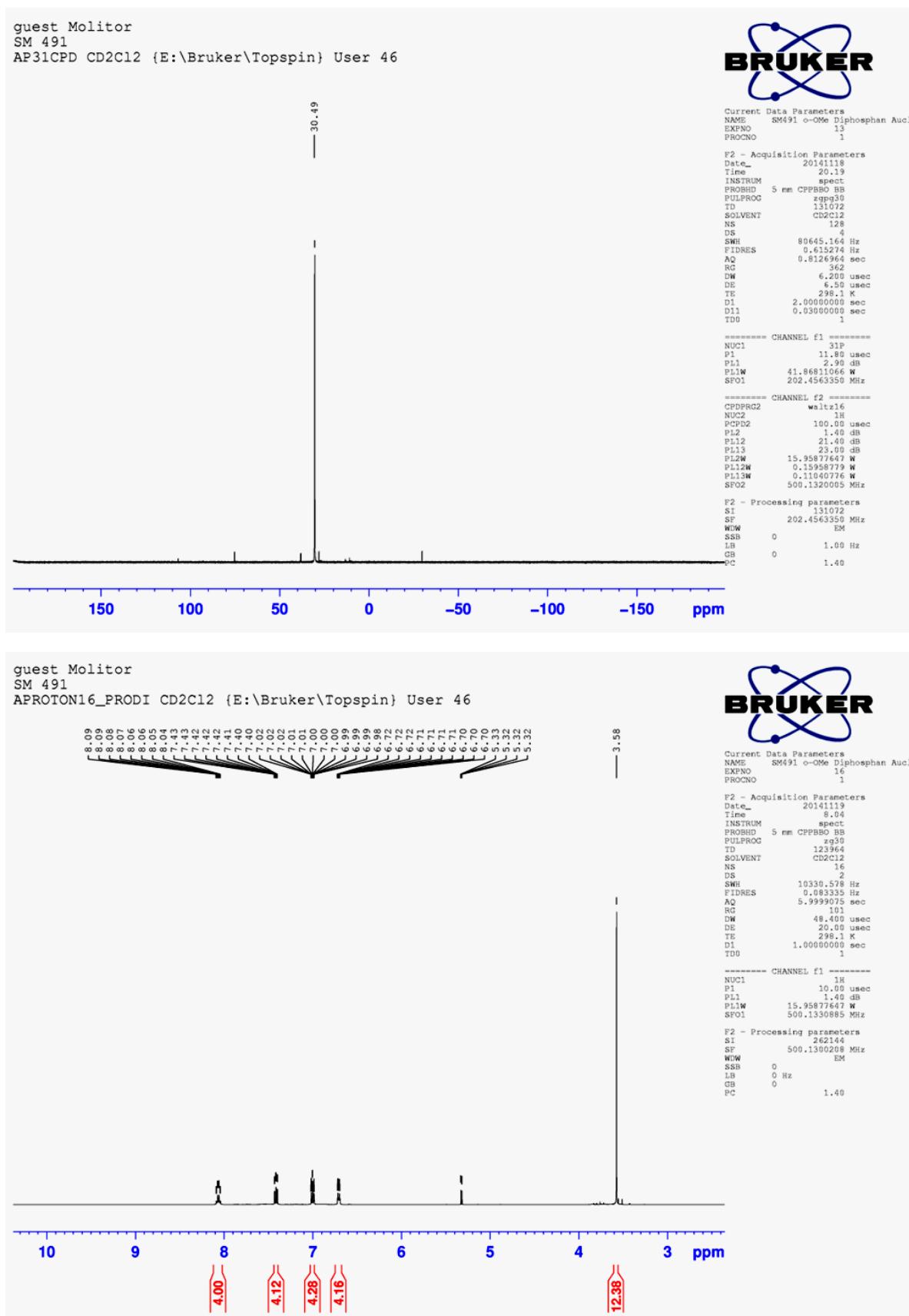


Figure S3b.  $^{13}\text{C}\{^1\text{H}\}$  NMR and  $^{13}\text{C}\{^1\text{H}\}$  DEPT135 NMR spectra of **2c**.

**Figure S4a.**  $^{31}\text{P}\{\text{H}\}$  NMR and  $^1\text{H}$  NMR spectra of **2d**.

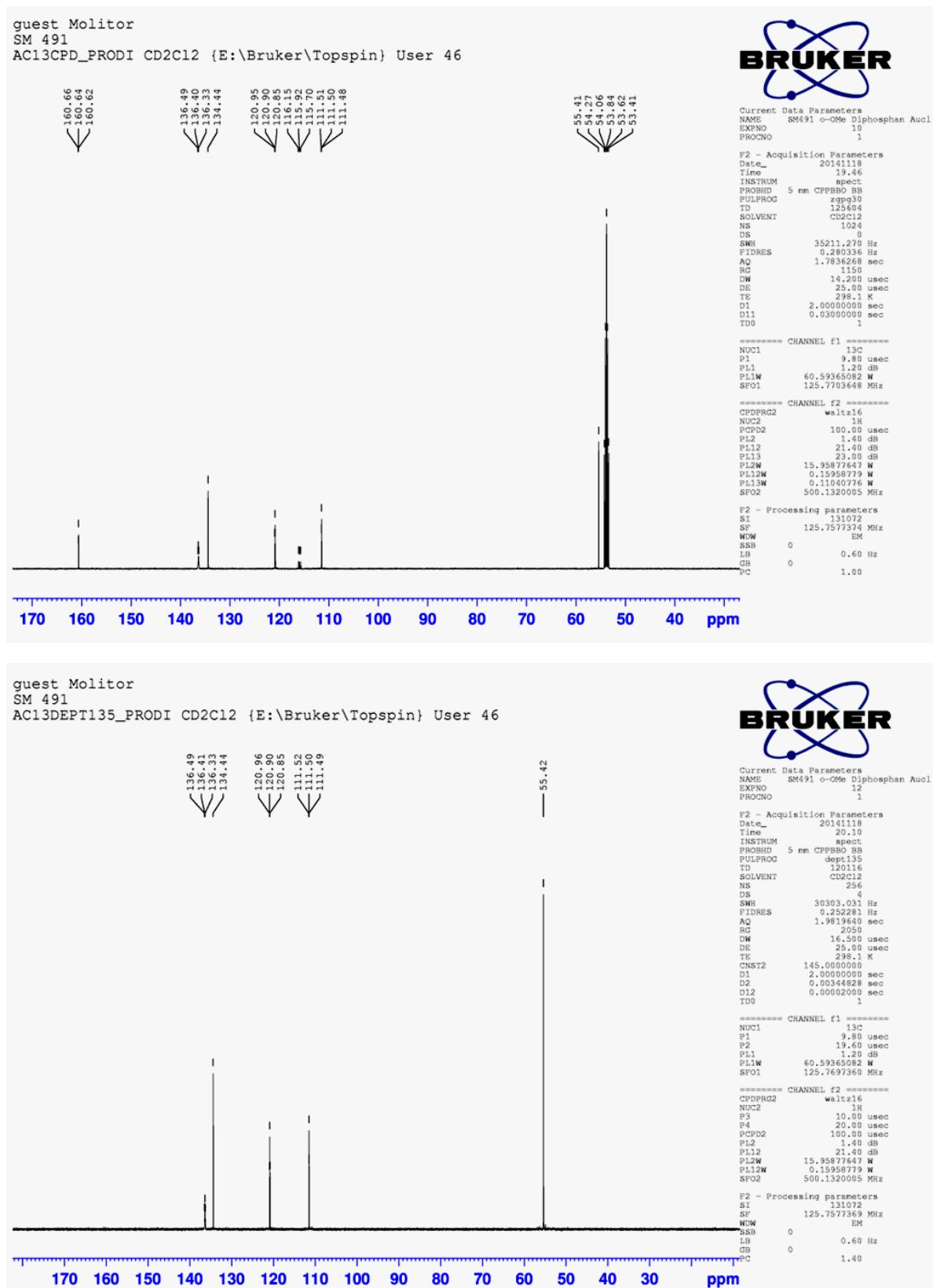


Figure S4b.  $^{13}\text{C}\{\text{H}\}$  NMR and  $^{13}\text{C}\{\text{H}\}$  DEPT135 NMR spectra of **2d**.

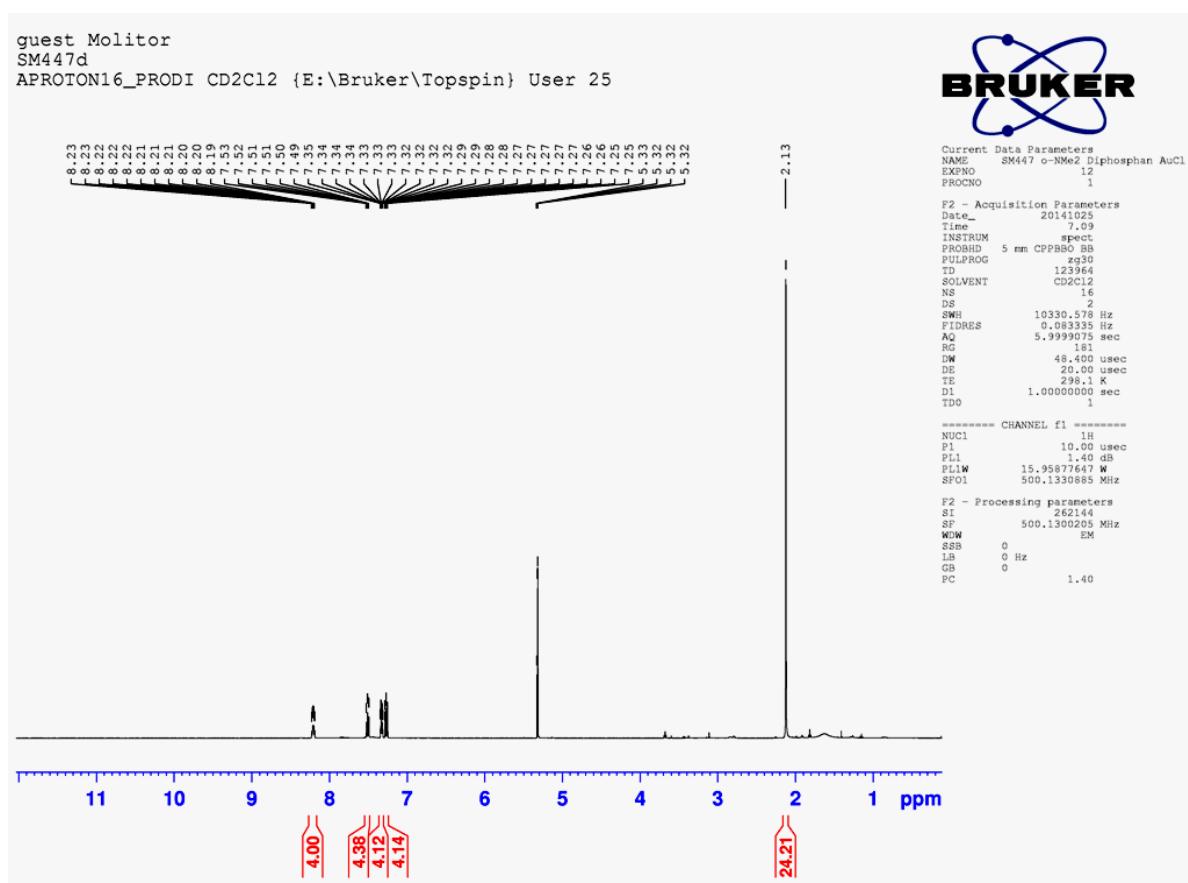
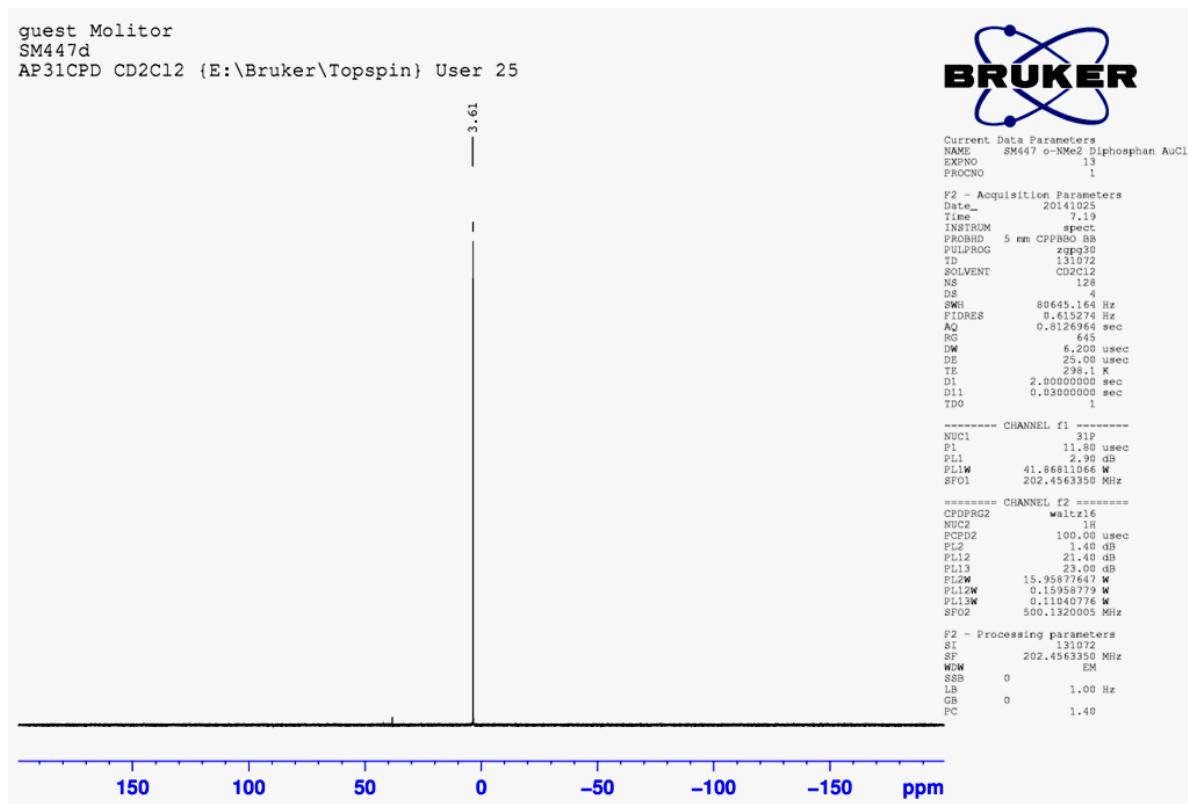
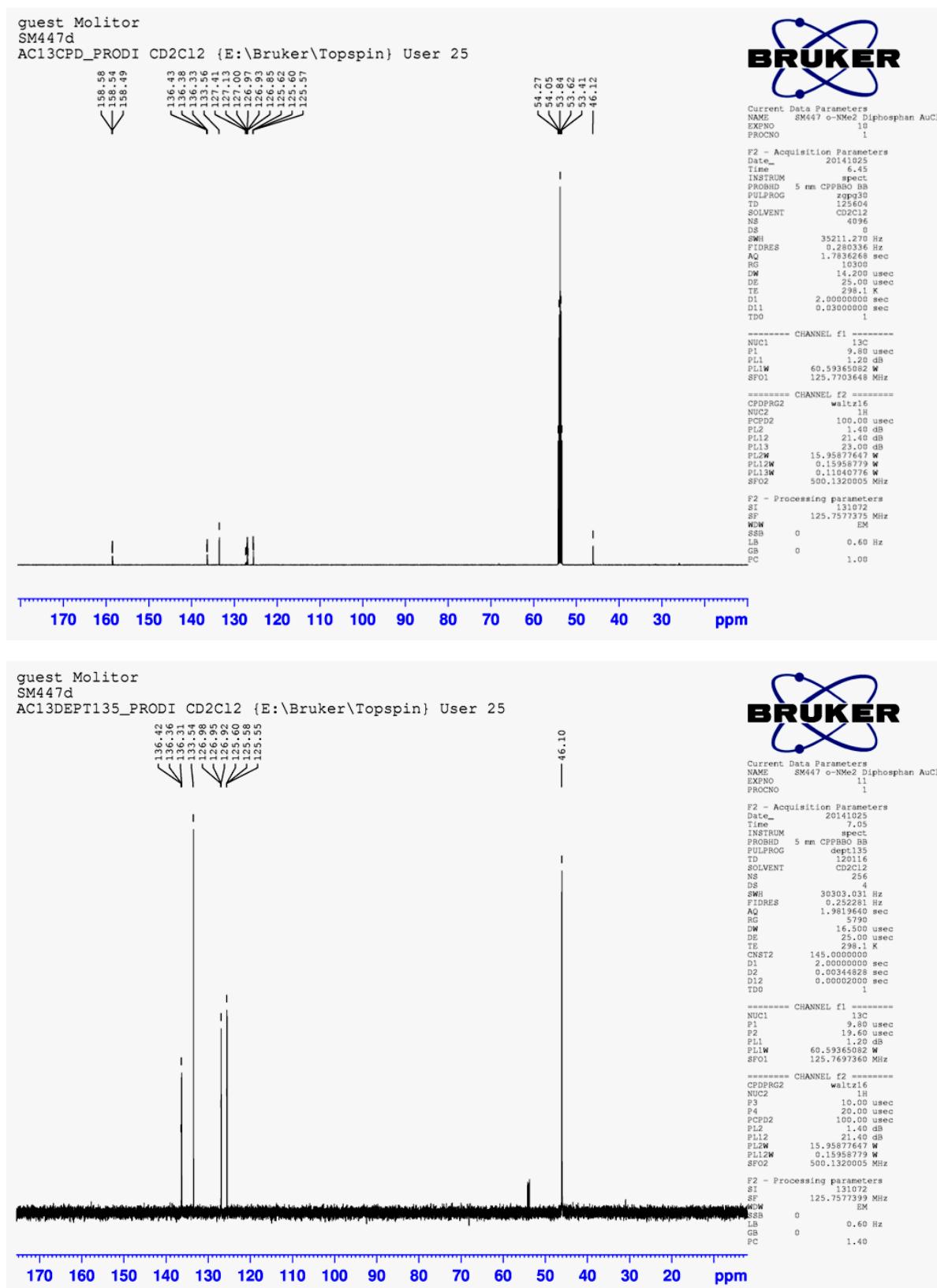


Figure S5a.  $^{31}\text{P}\{\text{H}\}$  NMR and  $^1\text{H}$  NMR spectra of **2e**.



**Figure S5b.**  $^{13}\text{C}\{^1\text{H}\}$  NMR and  $^{13}\text{C}\{^1\text{H}\}$  DEPT135 NMR spectra of **2e**.

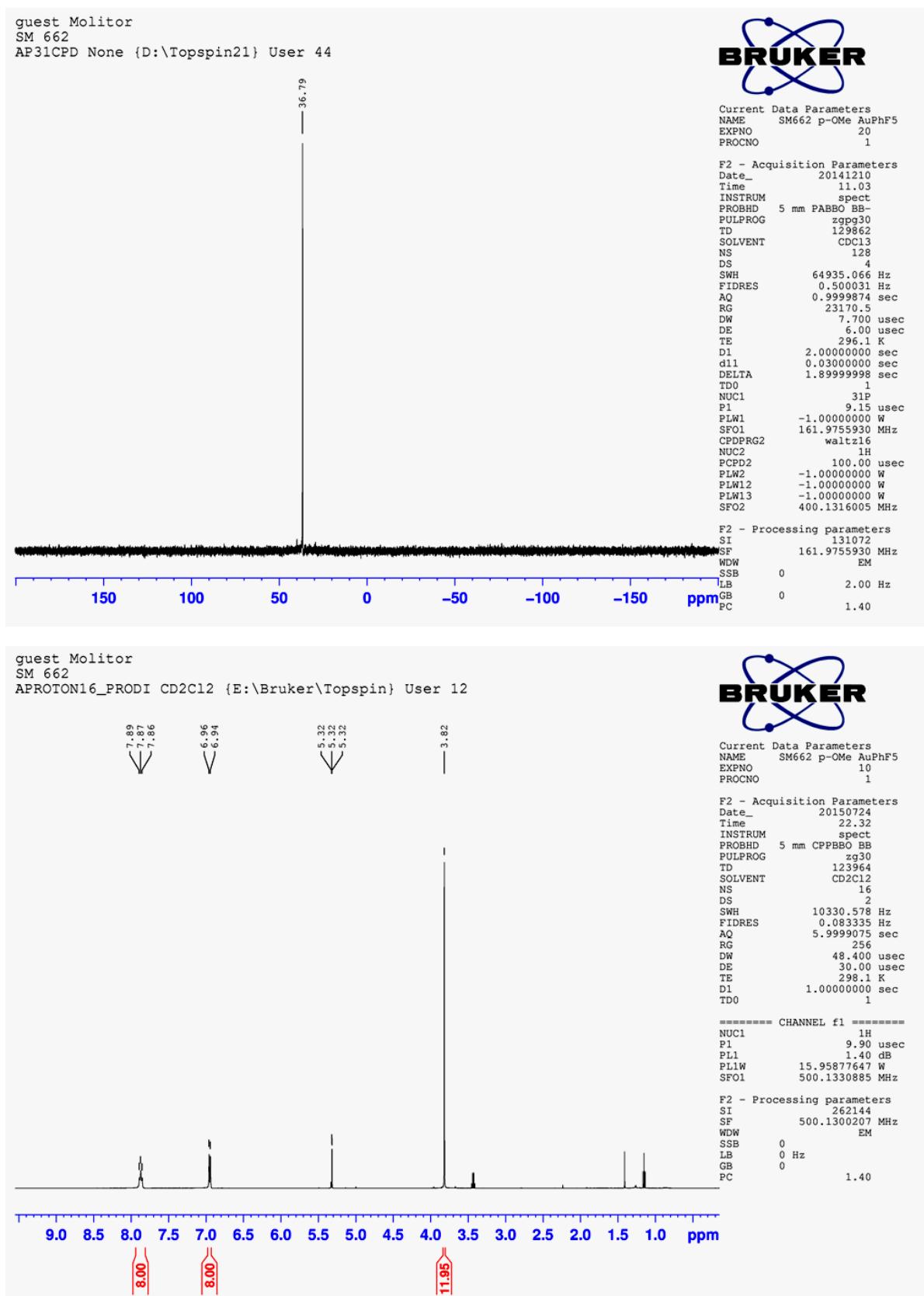


Figure S6a.  $^{31}\text{P}\{\text{H}\}$  NMR and  $^1\text{H}$  NMR spectra of **2h**.

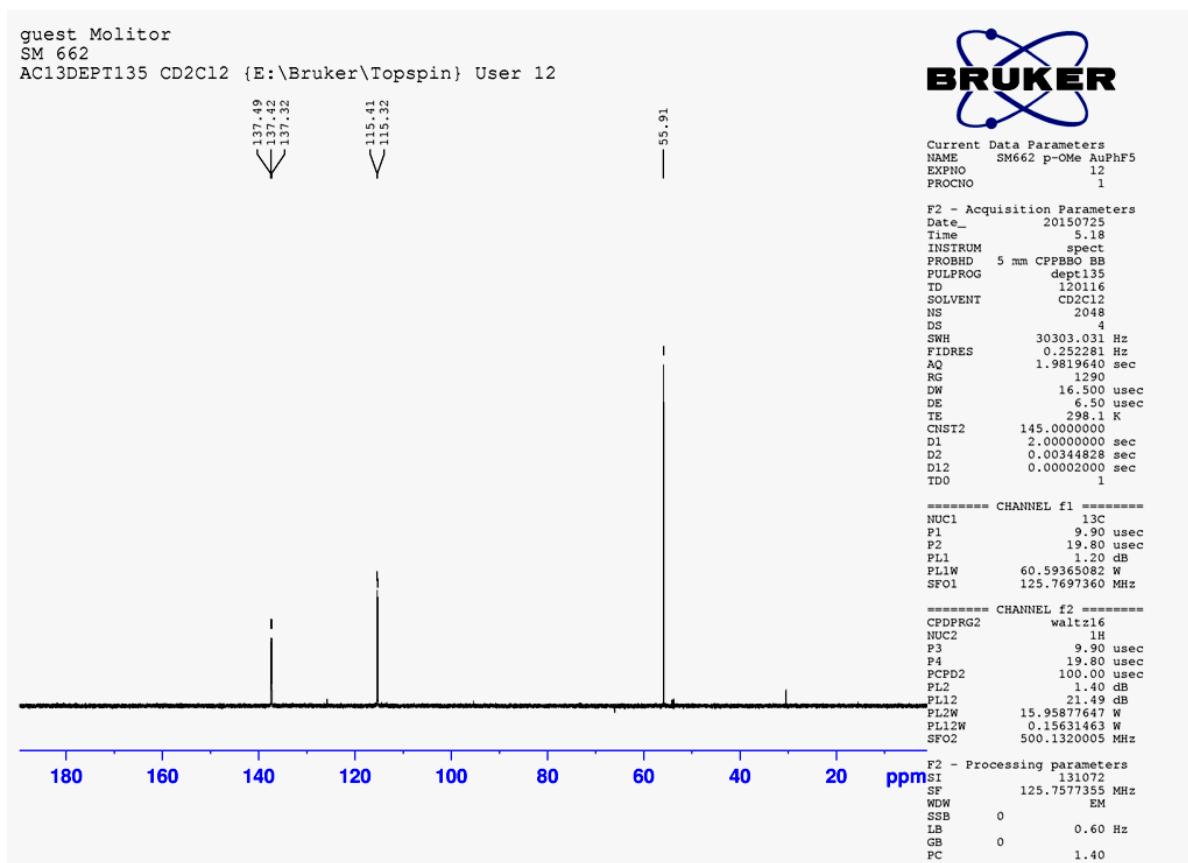
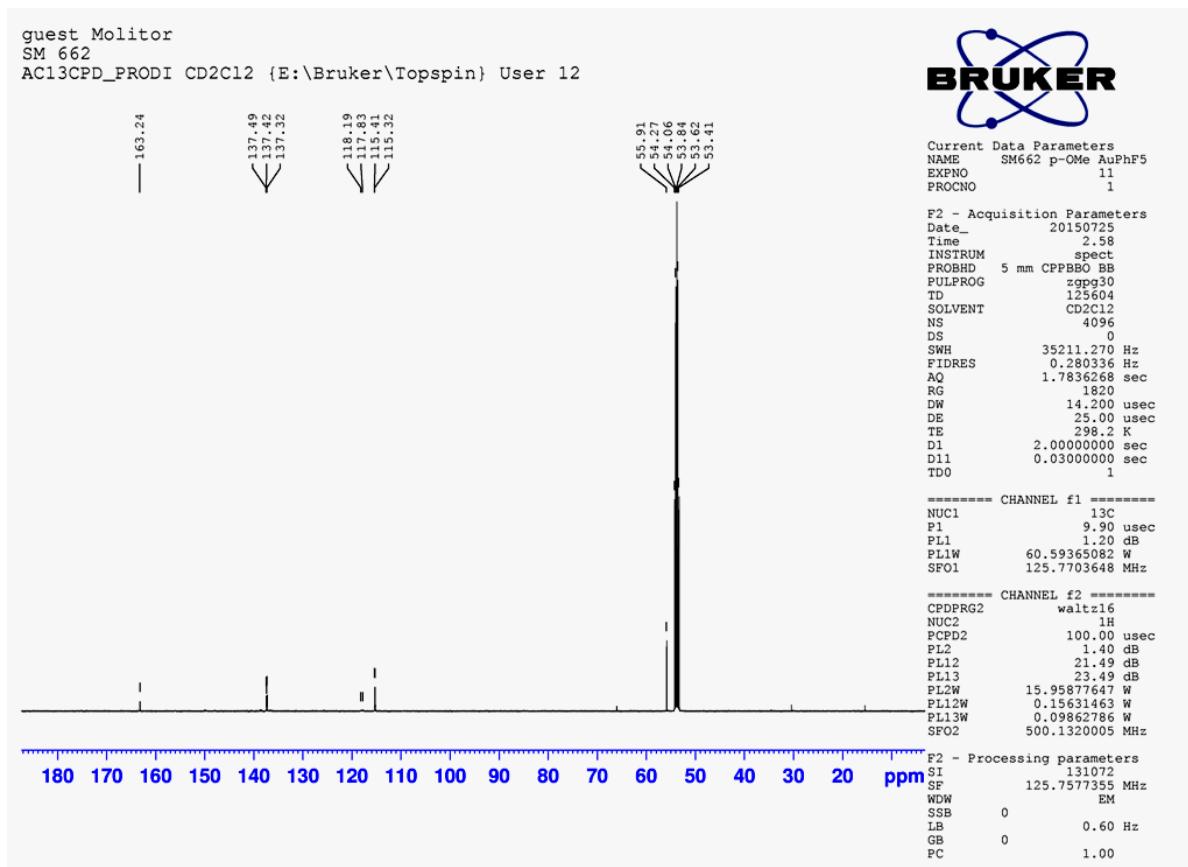


Figure S6b.  $^{13}\text{C}\{^1\text{H}\}$  NMR and  $^{13}\text{C}\{^1\text{H}\}$  DEPT135 NMR spectra of **2h**.

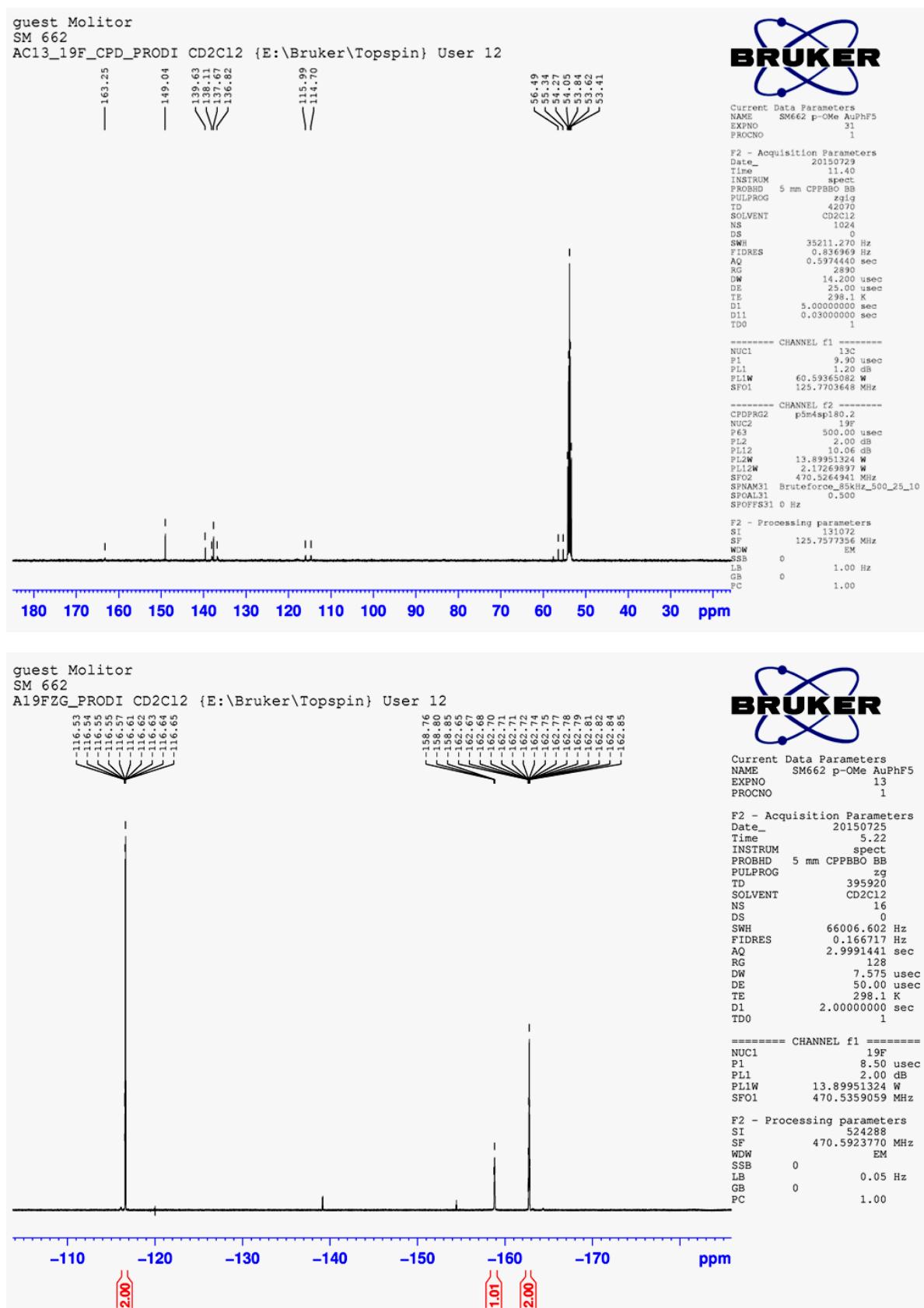


Figure S6c.  $^{13}\text{C}\{^{19}\text{F}\}$  NMR and  $^{19}\text{F}\{^1\text{H}\}$  NMR spectra of **2h**.

## 2. Crystal Structure Determination

Data collection of all compounds was conducted with a Bruker APEX2-CCD (D8 three-circle goniometer). The structures were solved using direct methods, refined with the Shelx software package<sup>[1]</sup> and expanded using Fourier techniques. The crystals of all compounds were mounted in an inert oil (perfluoropolyalkylether). Crystal structure determinations were effected at 100 K. Crystallographic data (excluding structure factors) have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-1463741-1463748. Copies of the data can be obtained free of charge on application to Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; [fax: (+44) 1223-336-033; email: deposit@ccdc.cam.ac.uk].

**Table S1.** Data collection and structure refinement details for compounds **2a-2c**.

Compound	<b>1d</b>	<b>1f</b>
CCDC No.	CCDC-1463741	CCDC-1463742
Formula	C <sub>28</sub> H <sub>28</sub> O <sub>4</sub> P <sub>2</sub>	C <sub>28</sub> H <sub>28</sub> P <sub>2</sub>
Formula weight [g·mol <sup>-1</sup> ]	490.44	426.44
Temperature [K]	100(2)	100(2)
Wave length [Å]	0.71073	0.71073
Crystal system	monoclinic	monoclinic
Space group	C2/c (15)	P2 <sub>1</sub> /c (14)
a [Å]	14.3337(13)	7.5386(3)
b [Å]	8.0972(7)	16.2636(7)
c [Å]	21.2171(19)	18.9268(8)
β [°]	91.838(3)	100.154(1)
Volume [Å <sup>3</sup> ]	2461.2(4)	2284.17(17)
Z	4	4
Calc. density [Mg·m <sup>-3</sup> ]	1.324	1.240
μ (Mo <sub>Kα</sub> ) [mm <sup>-1</sup> ]	0.210	0.203
F(000)	1032	904
Crystal dimensions [mm]	0.26 x 0.16 x 0.04	0.26 x 0.21 x 0.13
Theta range [°]	2.89 to 26.42	1.66 to 26.44
Index ranges	-17 ≤ k ≤ 17 -10 ≤ k ≤ 10 -26 ≤ k ≤ 26	-9 ≤ h ≤ 9 -20 ≤ k ≤ 20 -23 ≤ l ≤ 23
Reflections collected	15540	30184
Independent reflections	2523 [ <i>R</i> <sub>int</sub> = 0.0578]	4701 [ <i>R</i> <sub>int</sub> = 0.0403]
Data/Restraints/Parameter	2523 / 0 / 146	4701 / 0 / 275
Goodness-of-fit on F <sup>2</sup>	1.035	1.010
Final R indices [I>2sigma(I)]	<i>R</i> 1 = 0.0431 w <i>R</i> 2 = 0.01095	<i>R</i> 1 = 0.0326 w <i>R</i> 2 = 0.0789
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0545 w <i>R</i> 2 = 0.1157	<i>R</i> 1 = 0.0431 w <i>R</i> 2 = 0.0871
Largest diff. peak and hole	0.476 and -0.335	0.307 and -0.237

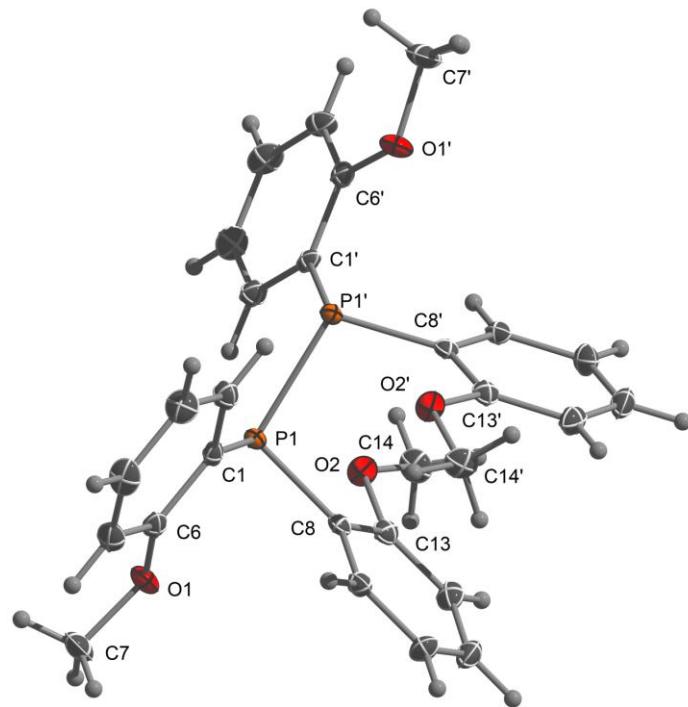
**Table S2.** Data collection and structure refinement details for compounds **2a-2c**.

Compound	<b>2a</b>	<b>2b</b>	<b>2c</b>
CCDC No.	CCDC-1463743	CCDC-1463744	CCDC-1463745
Formula	C <sub>28</sub> H <sub>28</sub> Au <sub>2</sub> Cl <sub>2</sub> P <sub>2</sub>	C <sub>28</sub> H <sub>28</sub> Au <sub>2</sub> Cl <sub>2</sub> O <sub>4</sub> P <sub>2</sub>	C <sub>34</sub> H <sub>44</sub> Au <sub>2</sub> Cl <sub>6</sub> N <sub>4</sub> P <sub>2</sub>
Formula weight [g·mol <sup>-1</sup> ]	891.28	955.28	1177.31
Temperature [K]	100(2)	100(2)	100(2)
Wave length [Å]	0.71073	0.71073	0.71073
Crystal system	orthorhombic	monoclinic	triclinic
Space group	<i>Pca2</i> <sub>1</sub> (29)	<i>C2/c</i> (15)	<i>P-1</i> (2)
a [Å]	11.5429(8)	15.401(2)	10.3579(9)
b [Å]	16.0408(11)	12.9857(19)	10.4563(7)
c [Å]	14.5815(11)	14.468(3)	11.1637(7)
α [°]			62.997(2)
β [°]		100.885(6)	68.316(2)
γ [°]			78.142(2)
Volume [Å <sup>3</sup> ]	2699.8(3)	2841.4(8)	1000.00(11)
Z	4	4	1
Calc. density [Mg·m <sup>-3</sup> ]	2.193	2.233	1.955
μ (Mo <sub>Kα</sub> ) [mm <sup>-1</sup> ]	11.188	10.649	7.838
F(000)	1672	1800	566
Crystal dimensions [mm]	0.34 x 0.22 x 0.17	0.16 x 0.12 x 0.08	0.19 x 0.15 x 0.03
Theta range [°]	1.27 to 24.99	3.32 to 25.00	3.65 to 25.00
Index ranges	-13 ≤ k ≤ 13 -19 ≤ k ≤ 19 -17 ≤ k ≤ 17	-18 ≤ h ≤ 16 -15 ≤ k ≤ 15 -17 ≤ l ≤ 17	-12 ≤ h ≤ 12 -11 ≤ k ≤ 12 -13 ≤ l ≤ 11
Reflections collected	31069	11261	8676
Independent reflections	4745 [ <i>R</i> <sub>int</sub> = 0.0553]	2502 [ <i>R</i> <sub>int</sub> = 0.0403]	3508 [ <i>R</i> <sub>int</sub> = 0.0352]
Data/Restraints/Parameter	4745 / 1 / 251	2502 / 0 / 174	3508 / 0 / 221
Goodness-of-fit on F <sup>2</sup>	1.066	1.031	1.033
Final R indices [I>2sigma(I)]	<i>R</i> 1 = 0.0234 w <i>R</i> 2 = 0.0459	<i>R</i> 1 = 0.0209 w <i>R</i> 2 = 0.0386	<i>R</i> 1 = 0.0273 w <i>R</i> 2 = 0.0518
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0322 w <i>R</i> 2 = 0.0490	<i>R</i> 1 = 0.0285 w <i>R</i> 2 = 0.0412	<i>R</i> 1 = 0.0351 w <i>R</i> 2 = 0.0548
Largest diff. peak and hole	1.151 and -0.647	0.612 and -0.733	0.969 and -0.561

**Table S3.** Data collection and structure refinement details for compounds **2d**, **2e** and **2h**.

Compound	<b>2d</b>	<b>2e</b>	<b>2h</b>
CCDC No.	CCDC-1463746	CCDC-1463747	CCDC-1463748
Formula	C <sub>32</sub> H <sub>36</sub> Au <sub>2</sub> Cl <sub>2</sub> O <sub>5</sub> P <sub>2</sub>	C <sub>32</sub> H <sub>40</sub> Au <sub>2</sub> Cl <sub>2</sub> N <sub>4</sub> P <sub>2</sub>	C <sub>40</sub> H <sub>28</sub> Au <sub>2</sub> F <sub>10</sub> O <sub>4</sub> P <sub>2</sub>
Formula weight [g·mol <sup>-1</sup> ]	1027.38	1007.45	1218.50
Temperature [K]	100(2)	100(2)	100(2)
Wave length [Å]	0.71073	0.71073	0.71073
Crystal system	triclinic	triclinic	triclinic
Space group	<i>P</i> -1 (2)	<i>P</i> -1 (2)	<i>P</i> -1 (2)
a [Å]	10.9838(5)	11.4972(5)	7.3242(5)
b [Å]	12.5329(6)	15.3421(7)	11.2949(8)
c [Å]	13.3045(6)	21.1914(10)	13.0454(9)
α [°]	77.741(2)	94.108(2)	110.027(2)
β [°]	80.078(2)	90.027(2)	105.628(2)
γ [°]	75.775(2)	92.970(2)	93.035(2)
Volume [Å <sup>3</sup> ]	1720.84(14)	3723.3(3)	963.80(12)
Z	2	4	1
Calc. density [Mg·m <sup>-3</sup> ]	1.983	1.797	2.099
μ (Mo <sub>Kα</sub> ) [mm <sup>-1</sup> ]	8.801	8.127	7.776
F(000)	980	1928	578
Crystal dimensions [mm]	0.23 x 0.09 x 0.06	0.26 x 0.14 x 0.03	0.15 x 0.11 x 0.02
Theta range [°]	2.44 to 24.99	1.33 to 25.00	2.91 to 24.99
Index ranges	-13 ≤ k ≤ 13 -14 ≤ k ≤ 14 -15 ≤ k ≤ 15	-13 ≤ h ≤ 13 -18 ≤ k ≤ 18 -25 ≤ l ≤ 25	-8 ≤ h ≤ 8 -13 ≤ k ≤ 13 -15 ≤ l ≤ 15
Reflections collected	21898	41029	11518
Independent reflections	6032 [ <i>R</i> <sub>int</sub> = 0.0481]	13083 [ <i>R</i> <sub>int</sub> = 0.0936]	3400 [ <i>R</i> <sub>int</sub> = 0.0304]
Data/Restraints/Parameter	6032 / 0 / 368	13083 / 0 / 767	3400 / 0 / 246
Goodness-of-fit on F <sup>2</sup>	1.025	1.055	1.087
Final R indices [I>2sigma(I)]	<i>R</i> 1 = 0.0364 w <i>R</i> 2 = 0.0832	<i>R</i> 1 = 0.0488 w <i>R</i> 2 = 0.0790	<i>R</i> 1 = 0.0226 w <i>R</i> 2 = 0.0522
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0536 w <i>R</i> 2 = 0.0909	<i>R</i> 1 = 0.0918 w <i>R</i> 2 = 0.0911	<i>R</i> 1 = 0.0247 w <i>R</i> 2 = 0.0530
Largest diff. peak and hole	2.286 and -1.777	1.09 and -1.208	2.087 and -0.863

## 2.1 Crystal Structure Determination of **1d**



**Figure S7.** ORTEP Plot of compound **1d**. Ellipsoids are drawn at the 50% probability level.

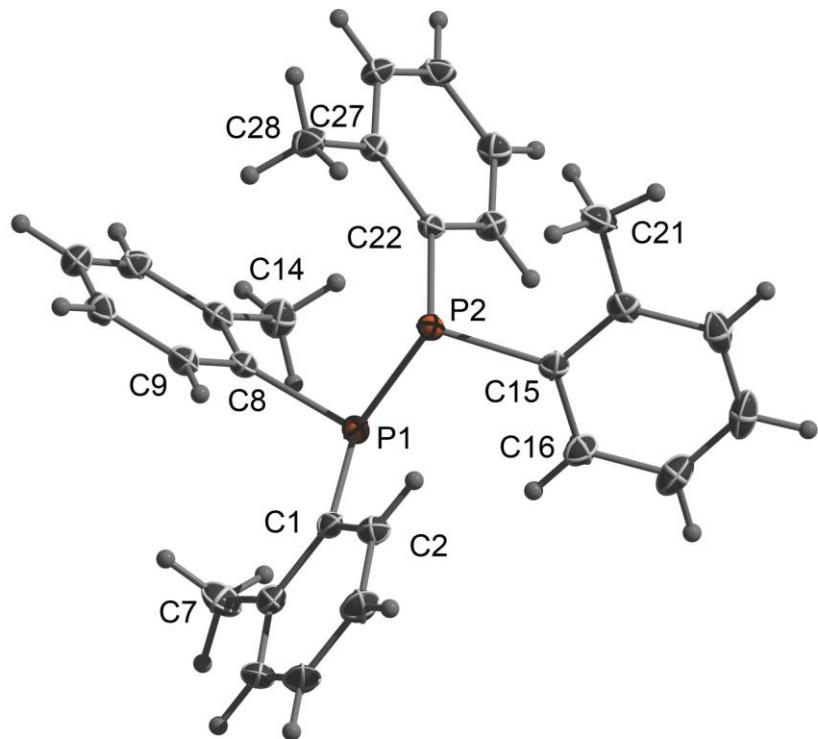
**Table S4.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for compound **1d**. U(eq) is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	U(eq)
P(1)	4533(1)	602(1)	2907(1)	11(1)
C(1)	5327(1)	1308(2)	3551(1)	13(1)
O(1)	4005(1)	1098(2)	4170(1)	19(1)
O(2)	3414(1)	-1657(2)	2170(1)	17(1)
C(2)	6256(1)	1777(2)	3492(1)	17(1)
C(3)	6770(2)	2491(3)	3992(1)	22(1)
C(4)	6348(2)	2746(3)	4562(1)	23(1)
C(5)	5426(2)	2285(3)	4641(1)	20(1)
C(6)	4920(1)	1576(2)	4140(1)	15(1)
C(7)	3513(2)	1521(3)	4720(1)	24(1)
C(8)	4369(1)	-1585(2)	3085(1)	13(1)
C(9)	4771(1)	-2376(3)	3609(1)	15(1)
C(10)	4615(2)	-4039(3)	3724(1)	19(1)
C(11)	4042(2)	-4934(3)	3313(1)	21(1)
C(12)	3628(1)	-4184(3)	2786(1)	19(1)
C(13)	3787(1)	-2521(3)	2675(1)	15(1)
C(14)	2938(2)	-2584(3)	1684(1)	21(1)

**Table S5.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for compound **1d**. The anisotropic displacement factor exponent takes the form:  $-2p^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^{*} b^{*} U^{12} ]$ .

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
P(1)	13(1)	11(1)	9(1)	-1(1)	1(1)	0(1)
C(1)	17(1)	10(1)	11(1)	0(1)	-2(1)	2(1)
O(1)	19(1)	25(1)	12(1)	-2(1)	5(1)	2(1)
O(2)	18(1)	17(1)	15(1)	0(1)	-5(1)	-1(1)
C(2)	19(1)	16(1)	15(1)	-2(1)	0(1)	0(1)
C(3)	19(1)	24(1)	23(1)	-2(1)	-4(1)	-3(1)
C(4)	28(1)	23(1)	17(1)	-4(1)	-9(1)	1(1)
C(5)	29(1)	19(1)	12(1)	0(1)	-2(1)	5(1)
C(6)	20(1)	12(1)	12(1)	1(1)	-1(1)	2(1)
C(7)	26(1)	31(1)	17(1)	-1(1)	9(1)	7(1)
C(8)	11(1)	14(1)	13(1)	0(1)	5(1)	1(1)
C(9)	17(1)	16(1)	12(1)	-2(1)	2(1)	-1(1)
C(10)	23(1)	17(1)	18(1)	5(1)	0(1)	3(1)
C(11)	21(1)	12(1)	29(1)	2(1)	4(1)	0(1)
C(12)	16(1)	16(1)	24(1)	-3(1)	2(1)	-4(1)
C(13)	11(1)	16(1)	17(1)	1(1)	3(1)	1(1)
C(14)	19(1)	25(1)	17(1)	-4(1)	-5(1)	-4(1)

## 2.2 Crystal Structure Determination of **1f**



**Figure S8.** ORTEP Plot of compound **1f**. Ellipsoids are drawn at the 50% probability level.

**Table S6.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for compound **1f**. U(eq) is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

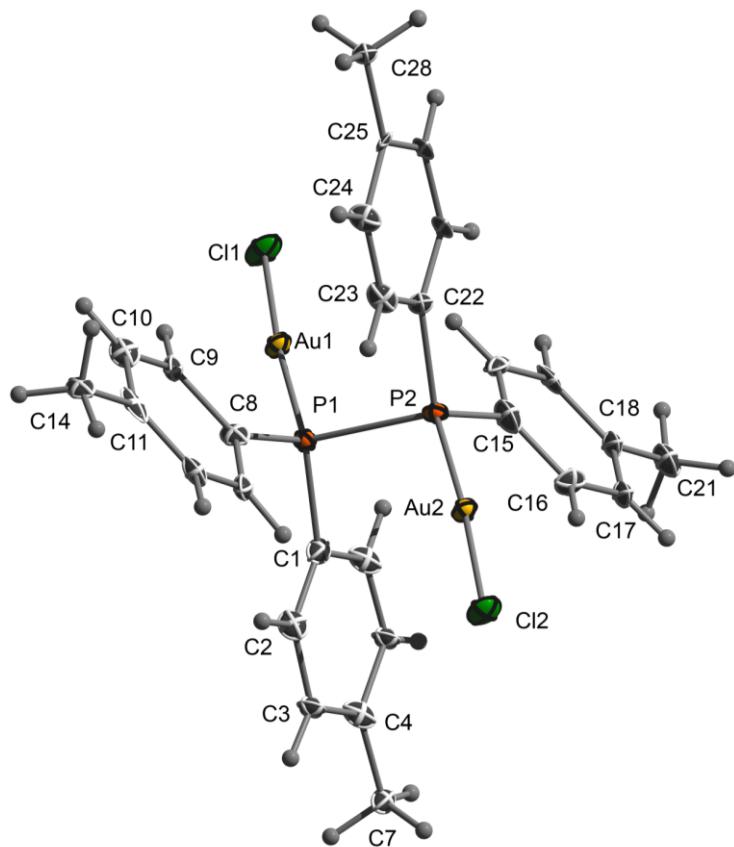
	x	y	z	U(eq)
P(1)	733(1)	7363(1)	3163(1)	14(1)
C(1)	-1570(2)	7012(1)	2796(1)	15(1)
P(2)	886(1)	7142(1)	4335(1)	14(1)
C(2)	-2653(2)	6582(1)	3196(1)	20(1)
C(3)	-4393(2)	6342(1)	2893(1)	25(1)
C(4)	-5076(2)	6548(1)	2191(1)	27(1)
C(5)	-4002(2)	6960(1)	1782(1)	23(1)
C(6)	-2235(2)	7179(1)	2068(1)	18(1)
C(7)	-1076(2)	7588(1)	1594(1)	23(1)
C(8)	333(2)	8488(1)	3169(1)	14(1)
C(9)	-1344(2)	8800(1)	3258(1)	17(1)
C(10)	-1678(2)	9639(1)	3243(1)	20(1)
C(11)	-324(2)	10178(1)	3137(1)	22(1)
C(12)	1335(2)	9879(1)	3042(1)	22(1)
C(13)	1698(2)	9035(1)	3051(1)	17(1)
C(14)	3533(2)	8748(1)	2939(1)	25(1)
C(15)	1736(2)	6079(1)	4418(1)	16(1)
C(16)	1729(2)	5576(1)	3819(1)	21(1)
C(17)	2237(2)	4755(1)	3890(1)	27(1)
C(18)	2746(2)	4425(1)	4568(1)	30(1)
C(19)	2747(2)	4913(1)	5167(1)	28(1)
C(20)	2244(2)	5738(1)	5110(1)	21(1)
C(21)	2281(3)	6241(1)	5781(1)	30(1)
C(22)	2948(2)	7755(1)	4625(1)	15(1)
C(23)	4634(2)	7473(1)	4518(1)	17(1)
C(24)	6176(2)	7944(1)	4716(1)	19(1)
C(25)	6042(2)	8709(1)	5026(1)	22(1)
C(26)	4380(2)	8988(1)	5146(1)	19(1)
C(27)	2818(2)	8526(1)	4953(1)	16(1)
C(28)	1052(2)	8864(1)	5099(1)	22(1)

**Table S7.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for compound **1f**. The anisotropic displacement factor exponent takes the form:  $-2p^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^{*} b^{*} U^{12} ]$ .

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
P(1)	13(1)	12(1)	16(1)	2(1)	2(1)	0(1)
C(1)	15(1)	10(1)	19(1)	-2(1)	2(1)	1(1)
P(2)	13(1)	14(1)	16(1)	1(1)	2(1)	0(1)
C(2)	22(1)	19(1)	20(1)	-2(1)	5(1)	-2(1)
C(3)	20(1)	25(1)	32(1)	-8(1)	9(1)	-7(1)
C(4)	16(1)	27(1)	36(1)	-14(1)	-1(1)	-1(1)
C(5)	24(1)	20(1)	22(1)	-7(1)	-5(1)	5(1)
C(6)	22(1)	12(1)	19(1)	-3(1)	1(1)	3(1)
C(7)	34(1)	18(1)	16(1)	3(1)	1(1)	1(1)
C(8)	16(1)	12(1)	13(1)	2(1)	0(1)	-1(1)

C(9)	17(1)	16(1)	18(1)	1(1)	3(1)	-2(1)
C(10)	19(1)	17(1)	22(1)	-2(1)	3(1)	3(1)
C(11)	29(1)	12(1)	24(1)	1(1)	2(1)	1(1)
C(12)	24(1)	16(1)	24(1)	4(1)	1(1)	-7(1)
C(13)	15(1)	19(1)	16(1)	4(1)	0(1)	-2(1)
C(14)	17(1)	24(1)	34(1)	9(1)	7(1)	-2(1)
C(15)	13(1)	14(1)	23(1)	3(1)	2(1)	-2(1)
C(16)	23(1)	15(1)	22(1)	3(1)	0(1)	-2(1)
C(17)	31(1)	14(1)	35(1)	-3(1)	1(1)	-3(1)
C(18)	32(1)	11(1)	44(1)	7(1)	-6(1)	-2(1)
C(19)	27(1)	22(1)	32(1)	14(1)	-5(1)	-6(1)
C(20)	16(1)	22(1)	23(1)	6(1)	0(1)	-5(1)
C(21)	37(1)	34(1)	20(1)	8(1)	4(1)	0(1)
C(22)	15(1)	16(1)	13(1)	3(1)	1(1)	-1(1)
C(23)	18(1)	16(1)	15(1)	2(1)	2(1)	2(1)
C(24)	15(1)	24(1)	19(1)	4(1)	3(1)	2(1)
C(25)	19(1)	21(1)	23(1)	3(1)	1(1)	-6(1)
C(26)	23(1)	13(1)	21(1)	0(1)	2(1)	-1(1)
C(27)	18(1)	16(1)	15(1)	3(1)	2(1)	1(1)
C(28)	21(1)	20(1)	26(1)	-6(1)	4(1)	3(1)

### 2.3 Crystal Structure Determination of **2a**



**Figure S9.** ORTEP Plot of compound **2a**. Ellipsoids are drawn at the 50% probability level.

**Table S8.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for compound **2a**. U(eq) is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	U(eq)
Au(1)	5511(1)	2787(1)	5257(1)	13(1)
Au(2)	2017(1)	2207(1)	2655(1)	13(1)
Cl(1)	7205(2)	3363(1)	5752(2)	23(1)
Cl(2)	275(2)	1711(1)	2168(2)	21(1)
P(1)	3826(2)	2335(1)	4706(1)	11(1)
P(2)	3722(2)	2626(1)	3206(1)	11(1)
C(1)	2588(7)	2907(4)	5162(6)	14(1)
C(2)	1534(7)	2591(5)	5359(5)	15(1)
C(3)	626(7)	3106(5)	5663(6)	15(1)
C(4)	783(7)	3954(5)	5730(5)	15(1)
C(5)	1876(6)	4292(6)	5530(5)	15(1)
C(6)	2741(6)	3765(4)	5258(5)	15(1)
C(7)	-186(6)	4520(5)	6010(5)	14(1)
C(8)	3608(7)	1224(5)	4716(6)	14(2)
C(9)	4527(7)	719(5)	5006(4)	14(1)
C(10)	4489(9)	-131(5)	4932(7)	15(1)
C(11)	3501(7)	-528(5)	4574(5)	19(2)
C(12)	2586(13)	-39(4)	4293(9)	13(3)
C(13)	2622(7)	819(5)	4372(5)	14(1)
C(14)	3463(7)	-1458(5)	4500(6)	14(2)
C(15)	3959(8)	3749(6)	3168(6)	22(2)
C(16)	3043(7)	4224(5)	2852(5)	15(2)
C(17)	3113(9)	5097(5)	2882(7)	15(1)
C(18)	4069(7)	5493(5)	3255(6)	15(1)
C(19)	4983(14)	5001(4)	3567(10)	14(3)
C(20)	4932(7)	4143(5)	3540(5)	14(2)
C(21)	4124(8)	6427(5)	3318(6)	22(2)
C(22)	4933(6)	2034(5)	2751(6)	15(1)
C(23)	4724(6)	1193(5)	2568(5)	15(2)
C(24)	5601(6)	701(5)	2271(5)	15(2)
C(25)	6710(7)	999(5)	2136(5)	14(2)
C(26)	6922(7)	1868(6)	2334(6)	22(2)
C(27)	6047(6)	2358(5)	2605(6)	22(2)
C(28)	7669(6)	426(5)	1791(5)	15(1)

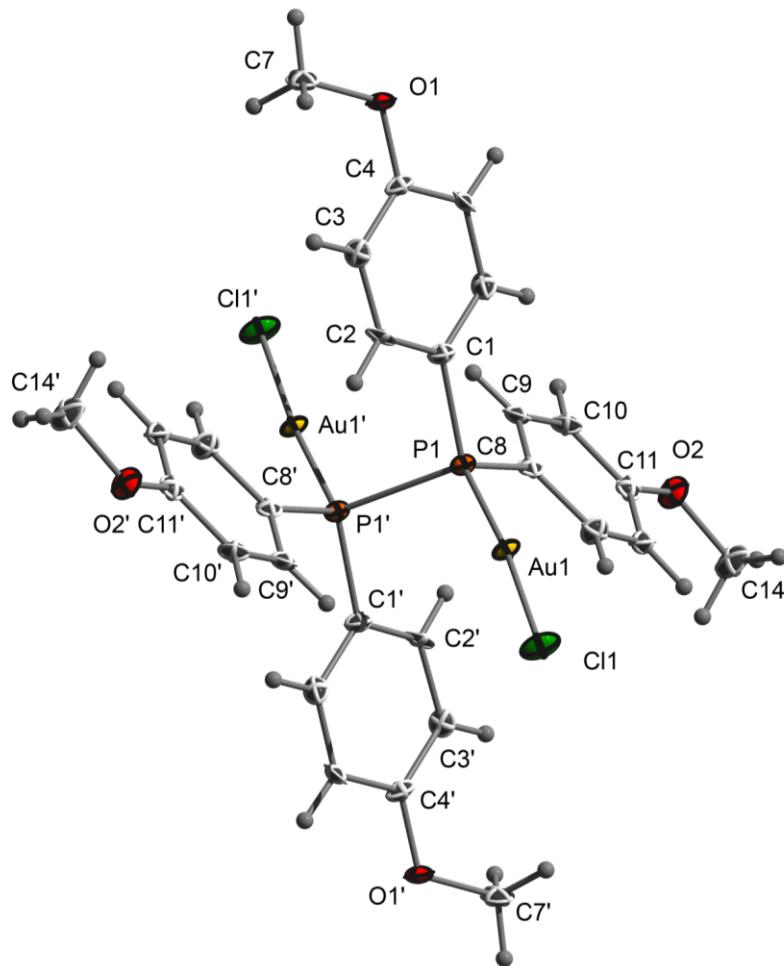
**Table S9.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for compound **2a**. The anisotropic displacement factor exponent takes the form:  $-2p^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$ .

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
Au(1)	11(1)	13(1)	16(1)	1(1)	-3(1)	-1(1)
Au(2)	11(1)	14(1)	14(1)	0(1)	-1(1)	0(1)
Cl(1)	16(1)	17(1)	35(1)	0(1)	-9(1)	-2(1)
Cl(2)	14(1)	22(1)	25(1)	-1(1)	-7(1)	-3(1)
P(1)	11(1)	12(1)	11(1)	1(1)	0(1)	-1(1)
P(2)	9(1)	11(1)	14(1)	0(1)	1(1)	-1(1)

C(1)	15(3)	16(3)	10(3)	-2(3)	-1(2)	4(3)
C(2)	21(3)	12(3)	13(3)	-5(3)	2(3)	0(3)
C(3)	8(3)	23(3)	13(3)	1(3)	1(2)	-2(2)
C(4)	15(3)	21(3)	10(3)	-7(3)	1(3)	-5(3)
C(5)	8(3)	23(3)	13(3)	1(3)	1(2)	-2(2)
C(6)	15(3)	21(3)	10(3)	-7(3)	1(3)	-5(3)
C(7)	15(3)	16(3)	10(3)	-2(3)	-1(2)	4(3)
C(8)	16(4)	9(3)	18(4)	-2(2)	6(3)	3(3)
C(9)	15(3)	16(3)	9(3)	4(2)	1(2)	3(3)
C(10)	21(3)	12(3)	13(3)	-5(3)	2(3)	0(3)
C(11)	36(5)	9(4)	12(4)	-1(3)	16(4)	2(4)
C(12)	17(7)	13(7)	10(7)	0(3)	2(5)	-6(3)
C(13)	15(3)	16(3)	9(3)	4(2)	1(2)	3(3)
C(14)	16(4)	9(3)	18(4)	-2(2)	6(3)	3(3)
C(15)	25(4)	21(4)	21(4)	7(3)	4(3)	-4(3)
C(16)	11(4)	21(4)	14(5)	-3(3)	-5(4)	-1(3)
C(17)	14(3)	13(3)	19(4)	8(2)	2(3)	0(2)
C(18)	14(3)	13(3)	19(4)	8(2)	2(3)	0(2)
C(19)	15(6)	17(7)	11(7)	2(3)	4(6)	-9(3)
C(20)	11(4)	18(4)	12(4)	-1(3)	1(3)	7(4)
C(21)	25(4)	21(4)	21(4)	7(3)	4(3)	-4(3)
C(22)	9(3)	19(3)	17(3)	6(3)	2(2)	3(2)
C(23)	15(4)	18(4)	12(4)	-3(4)	-2(3)	-8(3)
C(24)	15(4)	13(4)	17(4)	-4(3)	2(3)	-4(3)
C(25)	10(4)	20(4)	10(4)	7(3)	0(3)	10(3)
C(26)	10(3)	29(4)	27(3)	20(3)	7(3)	0(3)
C(27)	10(3)	29(4)	27(3)	20(3)	7(3)	0(3)
C(28)	9(3)	19(3)	17(3)	6(3)	2(2)	3(2)

---

## 2.4 Crystal Structure Determination of **2b**



**Figure S10.** ORTEP Plot of compound **2b**. Ellipsoids are drawn at the 50% probability level.

**Table S10.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for compound **2b**. U(eq) is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

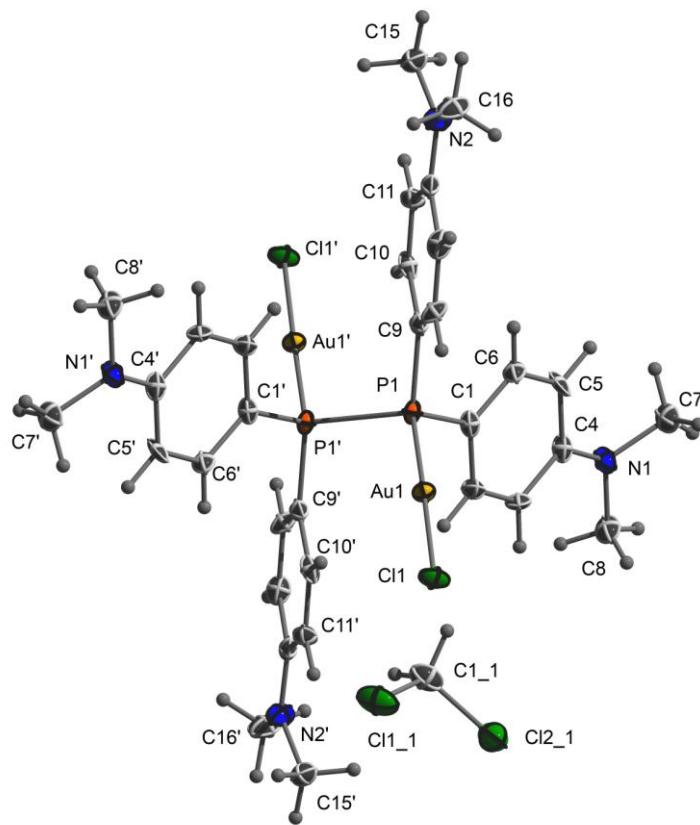
	x	y	z	U(eq)
Au(1)	544(1)	3714(1)	1576(1)	12(1)
Cl(1)	1371(1)	2403(1)	2346(1)	21(1)
P(1)	-179(1)	4985(1)	718(1)	10(1)
O(1)	-4103(2)	4692(2)	-245(2)	14(1)
C(1)	-1377(3)	4868(3)	472(3)	12(1)
O(2)	1021(2)	9190(2)	2000(2)	17(1)
C(2)	-1765(3)	4000(3)	8(3)	12(1)
C(3)	-2675(3)	3906(3)	-255(3)	11(1)
C(4)	-3210(3)	4685(3)	-6(3)	11(1)
C(5)	-2831(3)	5531(3)	513(3)	13(1)
C(6)	-1922(3)	5629(3)	733(3)	13(1)
C(7)	-4525(3)	3987(3)	-956(3)	17(1)
C(8)	130(3)	6253(3)	1153(3)	11(1)
C(9)	-286(3)	7150(3)	739(3)	13(1)
C(10)	22(3)	8109(3)	1048(3)	14(1)
C(11)	768(3)	8213(3)	1746(3)	12(1)
C(12)	1204(3)	7335(3)	2158(3)	13(1)

C(13)	873(3)	6369(3)	1868(3)	15(1)
C(14)	1831(3)	9341(3)	2655(3)	21(1)

**Table S11.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for compound **2b**. The anisotropic displacement factor exponent takes the form:  $-2p^2 [ h^2 a^*{}^2 U^{11} + \dots + 2 h k a^* b^* U^{12} ]$ .

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
Au(1)	10(1)	10(1)	13(1)	3(1)	0(1)	0(1)
Cl(1)	17(1)	16(1)	28(1)	9(1)	-2(1)	2(1)
P(1)	8(1)	11(1)	12(1)	1(1)	1(1)	0(1)
O(1)	6(2)	12(2)	21(2)	-5(1)	-1(1)	1(1)
C(1)	7(2)	14(2)	14(2)	1(2)	1(2)	0(2)
O(2)	18(2)	11(2)	22(2)	-4(1)	-2(1)	-3(2)
C(2)	10(2)	12(2)	14(2)	5(2)	6(2)	8(2)
C(3)	14(2)	6(2)	13(2)	0(2)	2(2)	-1(2)
C(4)	7(2)	13(2)	13(2)	4(2)	0(2)	-2(2)
C(5)	12(2)	16(2)	11(2)	-1(2)	6(2)	5(2)
C(6)	14(2)	13(2)	13(2)	-2(2)	4(2)	-5(2)
C(7)	8(2)	20(3)	24(3)	-4(2)	4(2)	-3(2)
C(8)	7(2)	14(2)	13(2)	-2(2)	4(2)	-3(2)
C(9)	8(2)	15(2)	16(3)	-1(2)	5(2)	3(2)
C(10)	11(2)	12(2)	18(3)	1(2)	3(2)	4(2)
C(11)	12(3)	14(2)	11(2)	0(2)	5(2)	-2(2)
C(12)	10(2)	16(3)	13(2)	1(2)	2(2)	1(2)
C(13)	16(2)	14(2)	14(2)	3(2)	2(2)	2(2)
C(14)	19(3)	16(3)	27(3)	-5(2)	-3(2)	-5(2)

## 2.5 Crystal Structure Determination of **2c**



**Figure S11.** ORTEP Plot of compound **2c**. Ellipsoids are drawn at the 50% probability level.

**Table S12.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for compound **2c**. U(eq) is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

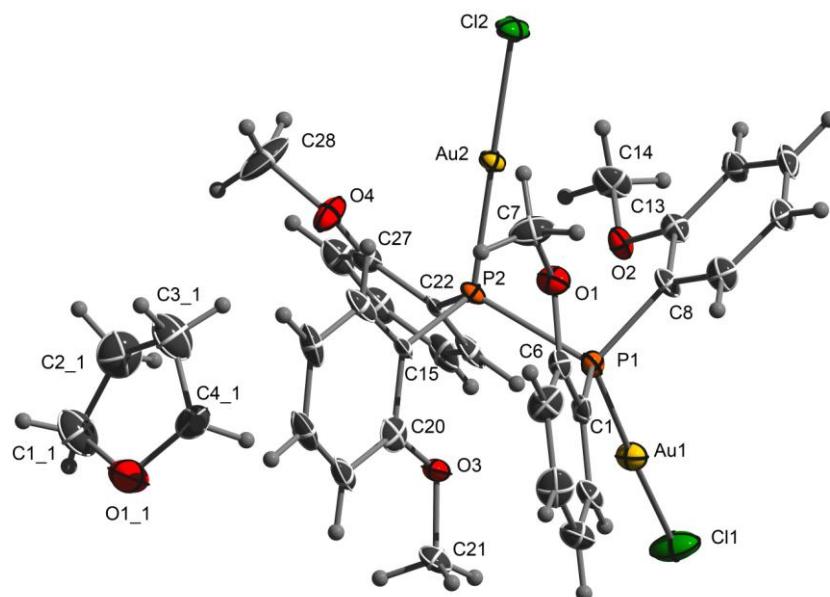
	x	y	z	U(eq)
Au(1)	7013(1)	1802(1)	2680(1)	15(1)
Cl(1)	9215(1)	2562(1)	1304(1)	23(1)
P(1)	4903(1)	962(1)	4023(1)	15(1)
N(1)	2468(4)	-1326(4)	1289(5)	20(1)
C(1)	4119(5)	280(5)	3236(5)	15(1)
N(2)	951(5)	5248(5)	5933(5)	23(1)
C(2)	4881(5)	-715(5)	2693(5)	18(1)
C(3)	4354(5)	-1228(6)	2034(5)	18(1)
C(4)	3010(5)	-766(5)	1899(5)	16(1)
C(5)	2273(5)	250(5)	2414(6)	19(1)
C(6)	2814(5)	756(5)	3074(5)	18(1)
C(7)	1396(5)	-492(6)	649(6)	25(1)
C(8)	3314(6)	-2333(6)	712(6)	24(1)
C(9)	3689(5)	2201(5)	4627(5)	15(1)
C(10)	2336(5)	1856(5)	5571(5)	15(1)
C(11)	1456(5)	2845(5)	6017(5)	18(1)
C(12)	1849(5)	4255(5)	5537(5)	18(1)
C(13)	3211(5)	4579(6)	4615(5)	20(1)
C(14)	4108(5)	3585(5)	4166(5)	18(1)

C(15)	-346(5)	4797(6)	7097(6)	26(1)
C(16)	1410(6)	6671(6)	5450(6)	28(1)
Cl11	13613(2)	4449(2)	155(2)	40(1)
C11	12282(6)	3943(6)	-135(6)	29(1)
Cl21	12802(2)	3865(2)	-1783(2)	38(1)

**Table S13.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for compound **2c**. The anisotropic displacement factor exponent takes the form:  $-2p^2[h^2a^{*2}U^{11} + \dots + 2hk a^* b^* U^{12}]$ .

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
Au(1)	14(1)	15(1)	15(1)	-6(1)	-4(1)	-2(1)
Cl(1)	15(1)	23(1)	28(1)	-10(1)	-2(1)	-3(1)
P(1)	16(1)	14(1)	14(1)	-5(1)	-5(1)	-2(1)
N(1)	22(2)	19(3)	26(3)	-12(2)	-13(2)	3(2)
C(1)	18(3)	14(3)	14(3)	-3(2)	-8(2)	-2(2)
N(2)	29(3)	16(2)	21(3)	-8(2)	-4(2)	0(2)
C(2)	13(3)	23(3)	17(3)	-10(2)	-4(2)	2(2)
C(3)	18(3)	20(3)	18(3)	-13(2)	-4(2)	6(2)
C(4)	22(3)	12(3)	15(3)	-3(2)	-9(2)	-4(2)
C(5)	20(3)	15(3)	29(3)	-11(2)	-18(2)	10(2)
C(6)	23(3)	16(3)	18(3)	-10(2)	-9(2)	3(2)
C(7)	26(3)	27(3)	30(3)	-16(3)	-14(3)	1(3)
C(8)	34(3)	21(3)	26(3)	-14(3)	-15(3)	3(3)
C(9)	16(3)	16(3)	15(3)	-6(2)	-9(2)	2(2)
C(10)	21(3)	8(3)	18(3)	-3(2)	-12(2)	-1(2)
C(11)	13(3)	21(3)	18(3)	-6(2)	-4(2)	-1(2)
C(12)	23(3)	19(3)	13(3)	-6(2)	-10(2)	2(2)
C(13)	26(3)	17(3)	18(3)	-6(2)	-8(2)	-5(2)
C(14)	20(3)	19(3)	16(3)	-10(2)	-2(2)	-5(2)
C(15)	24(3)	29(3)	19(3)	-10(3)	-2(2)	3(3)
C(16)	33(3)	21(3)	28(3)	-15(3)	-3(3)	0(3)
Cl11	26(1)	46(1)	64(1)	-35(1)	-15(1)	0(1)
C11	23(3)	24(3)	37(4)	-9(3)	-9(3)	-2(3)
Cl21	36(1)	42(1)	44(1)	-23(1)	-18(1)	8(1)

## 2.6 Crystal Structure Determination of **2d**



**Figure S12.** ORTEP Plot of compound **2d**. Ellipsoids are drawn at the 50% probability level.

**Table S14.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for compound **2d**. U(eq) is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	U(eq)
Au(1)	4620(1)	4678(1)	2928(1)	24(1)
Cl(1)	6141(3)	5620(2)	2967(2)	43(1)
P(1)	3121(2)	3785(2)	2821(2)	15(1)
O(1)	777(5)	2866(5)	3226(4)	22(1)
C(1)	1999(8)	3700(6)	3981(6)	17(2)
Au(2)	2507(1)	1806(1)	1393(1)	14(1)
Cl(2)	1198(2)	1611(2)	316(2)	24(1)
P(2)	3704(2)	2005(2)	2516(2)	14(1)
O(2)	4107(5)	3876(4)	716(4)	18(1)
C(2)	2213(8)	4071(7)	4828(6)	20(2)
O(3)	4668(5)	2088(5)	4407(4)	21(1)
C(3)	1439(8)	3970(7)	5770(7)	26(2)
O(4)	5026(5)	-74(5)	1923(5)	28(1)
C(4)	438(9)	3466(8)	5841(7)	30(2)
C(5)	186(8)	3083(7)	5028(7)	25(2)
C(6)	958(8)	3211(7)	4092(6)	22(2)
C(7)	-264(9)	2364(8)	3286(7)	34(2)
C(8)	2269(7)	4510(7)	1749(6)	17(2)
C(9)	1017(8)	5141(7)	1879(7)	23(2)
C(10)	440(8)	5747(7)	1033(7)	24(2)
C(11)	1088(8)	5704(7)	51(7)	25(2)
C(12)	2316(8)	5089(7)	-114(6)	22(2)
C(13)	2895(7)	4496(7)	744(6)	18(2)
C(14)	4757(8)	3627(8)	-264(6)	29(2)
C(15)	3390(7)	1197(6)	3793(6)	15(1)
C(16)	2587(8)	464(7)	3963(6)	24(1)

C(17)	2262(9)	-112(7)	4936(7)	28(2)
C(18)	2754(8)	65(7)	5766(6)	28(2)
C(19)	3564(8)	771(7)	5623(6)	26(2)
C(20)	3891(8)	1354(7)	4642(7)	23(2)
C(21)	5131(9)	2365(8)	5250(7)	29(2)
C(22)	5458(7)	1652(6)	2092(6)	15(1)
C(23)	6215(8)	2300(7)	2010(6)	24(1)
C(24)	7501(8)	2029(7)	1599(6)	27(2)
C(25)	7925(8)	1025(7)	1272(6)	25(1)
C(26)	7127(8)	302(8)	1354(6)	25(1)
C(27)	5866(8)	600(7)	1785(6)	22(2)
C(28)	5439(10)	-1091(9)	1509(10)	50(3)
O11	11565(7)	-1607(6)	3264(5)	47(2)
C21	12151(10)	-2045(10)	1590(8)	47(3)
C31	10765(10)	-1475(9)	1691(8)	46(2)
C41	10622(10)	-956(8)	2634(8)	38(2)
C11	12429(10)	-2365(10)	2677(8)	46(2)

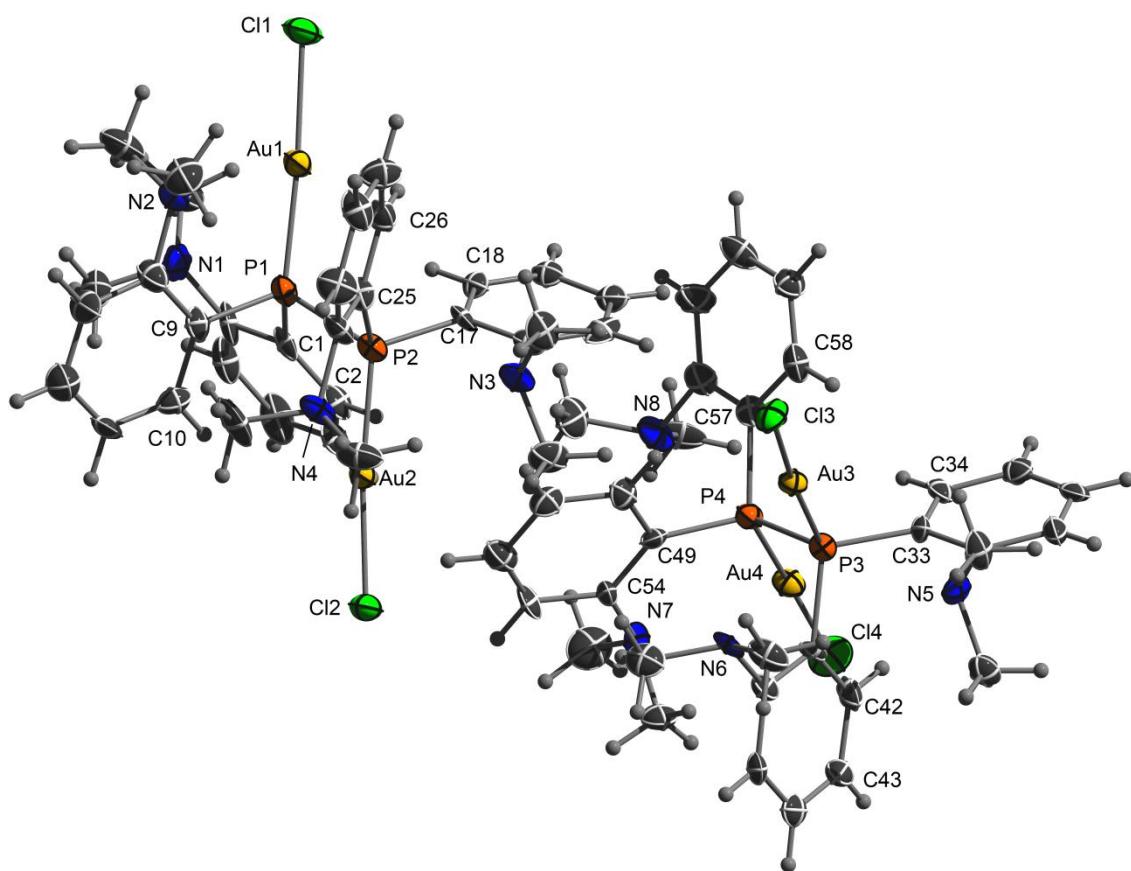
**Table S15.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for compound **2d**. The anisotropic displacement factor exponent takes the form:  $-2p^2 [ h^2 a^*{}^2 U^{11} + \dots + 2 h k a^* b^* U^{12} ]$ .

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
Au(1)	25(1)	26(1)	22(1)	-5(1)	-5(1)	-8(1)
Cl(1)	45(2)	56(2)	41(1)	-19(1)	-2(1)	-30(1)
P(1)	14(1)	16(1)	14(1)	-2(1)	-1(1)	-1(1)
O(1)	20(3)	27(3)	21(3)	-2(3)	-2(3)	-11(3)
C(1)	23(5)	11(4)	13(4)	3(3)	-1(3)	-4(3)
Au(2)	12(1)	17(1)	14(1)	-3(1)	-3(1)	-1(1)
Cl(2)	18(1)	31(1)	24(1)	-9(1)	-10(1)	0(1)
P(2)	10(1)	17(1)	13(1)	-1(1)	-3(1)	-2(1)
O(2)	14(3)	20(3)	15(3)	0(2)	1(2)	2(2)
C(2)	17(4)	21(4)	17(4)	1(3)	-5(3)	1(4)
O(3)	24(3)	24(3)	17(3)	-6(2)	-9(3)	-2(3)
C(3)	25(5)	33(5)	20(5)	-5(4)	-6(4)	-5(4)
O(4)	19(3)	21(3)	45(4)	-15(3)	-2(3)	-2(3)
C(4)	28(5)	34(5)	23(5)	-7(4)	11(4)	-3(4)
C(5)	18(5)	28(5)	27(5)	-8(4)	9(4)	-10(4)
C(6)	26(5)	16(4)	22(4)	-2(4)	-10(4)	2(4)
C(7)	28(5)	47(6)	35(5)	-18(5)	0(4)	-16(5)
C(8)	14(4)	20(4)	17(4)	1(3)	-5(3)	0(3)
C(9)	20(5)	25(5)	22(4)	-1(4)	1(4)	-6(4)
C(10)	20(5)	21(5)	31(5)	-5(4)	-11(4)	4(4)
C(11)	23(5)	17(4)	35(5)	6(4)	-16(4)	-2(4)
C(12)	28(5)	21(4)	16(4)	3(3)	-4(4)	-8(4)
C(13)	14(4)	21(4)	22(4)	1(4)	-4(3)	-8(4)
C(14)	26(5)	39(5)	17(4)	-7(4)	4(4)	-2(4)
C(15)	18(3)	14(3)	8(3)	0(2)	-5(2)	5(2)
C(16)	15(3)	30(3)	17(3)	2(3)	-4(3)	7(3)
C(17)	26(5)	22(5)	26(5)	10(4)	-2(4)	2(4)

C(18)	29(5)	29(5)	15(4)	6(4)	0(4)	6(4)
C(19)	30(5)	22(5)	18(4)	0(4)	-7(4)	10(4)
C(20)	14(4)	22(4)	28(5)	-8(4)	1(4)	8(4)
C(21)	28(5)	31(5)	29(5)	-4(4)	-17(4)	-2(4)
C(22)	18(3)	14(3)	8(3)	0(2)	-5(2)	5(2)
C(23)	15(3)	30(3)	17(3)	2(3)	-4(3)	7(3)
C(24)	28(5)	30(5)	24(5)	14(4)	-7(4)	-17(4)
C(25)	12(3)	35(4)	22(3)	-1(3)	2(3)	1(3)
C(26)	12(3)	35(4)	22(3)	-1(3)	2(3)	1(3)
C(27)	19(5)	28(5)	18(4)	-5(4)	-3(4)	-2(4)
C(28)	36(6)	45(6)	85(9)	-45(6)	4(6)	-18(5)
O11	63(5)	48(5)	38(4)	1(4)	-23(4)	-21(4)
C21	33(6)	54(7)	48(7)	-13(6)	7(5)	-5(5)
C31	28(4)	55(5)	49(5)	1(4)	-8(4)	-1(4)
C41	54(7)	27(5)	37(6)	-12(4)	-8(5)	-7(5)
C11	28(4)	55(5)	49(5)	1(4)	-8(4)	-1(4)

## 2.7 Crystal Structure Determination of **2e**

The molecular structure contained two strongly disordered DCM molecules. Refinement was done by using the squeeze routine in platon.<sup>2</sup>



**Figure S13.** ORTEP Plot of compound **2e**. Ellipsoids are drawn at the 50% probability level.

**Table S16.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for compound **2e**. U(eq) is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	U(eq)
Au(1)	11267(1)	2386(1)	3292(1)	30(1)
Au(2)	7485(1)	2367(1)	1508(1)	24(1)
Au(3)	13298(1)	2773(1)	-1485(1)	23(1)
Au(4)	16627(1)	2557(1)	-3462(1)	27(1)
Cl(1)	13024(3)	2714(2)	3804(2)	50(1)
Cl(2)	5726(2)	2132(2)	993(2)	35(1)
Cl(3)	11667(2)	3042(2)	-897(1)	32(1)
Cl(4)	18302(3)	2085(2)	-3928(2)	47(1)
P(1)	9568(3)	1979(2)	2828(1)	24(1)
P(2)	9186(2)	2740(2)	1995(1)	24(1)
P(3)	14881(2)	2408(2)	-2035(1)	22(1)
P(4)	15038(2)	3018(2)	-2964(1)	23(1)
N(1)	9283(8)	1018(6)	3928(4)	33(3)
N(2)	11610(8)	778(6)	2467(5)	34(3)
N(3)	9141(8)	4176(6)	1180(5)	31(2)
N(4)	9354(8)	1777(6)	668(4)	29(2)
N(5)	14995(7)	1143(5)	-1071(4)	23(2)
N(6)	15446(7)	3813(5)	-957(4)	22(2)
N(7)	17034(8)	4424(5)	-3099(4)	26(2)
N(8)	14471(8)	3746(6)	-4094(4)	35(3)
C(1)	8266(9)	2025(6)	3327(5)	22(3)
C(2)	7309(9)	2520(7)	3217(5)	29(2)
C(3)	6369(10)	2518(7)	3614(5)	29(2)
C(4)	6370(11)	2000(7)	4119(6)	44(4)
C(5)	7327(11)	1513(7)	4234(6)	39(3)
C(6)	8269(10)	1515(6)	3833(5)	29(3)
C(7)	8998(10)	67(7)	3897(6)	42(3)
C(8)	9916(10)	1276(8)	4509(5)	45(4)
C(9)	9471(9)	878(6)	2446(5)	24(3)
C(10)	8369(9)	484(7)	2296(5)	27(3)
C(11)	8263(10)	-366(7)	2023(5)	30(3)
C(12)	9207(11)	-831(8)	1882(6)	47(4)
C(13)	10307(10)	-451(7)	2012(6)	46(4)
C(14)	10467(10)	408(7)	2301(6)	32(3)
C(15)	12119(10)	363(8)	2984(6)	45(4)
C(16)	12376(10)	815(8)	1928(6)	48(4)
C(17)	9267(9)	3871(6)	2303(5)	22(3)
C(18)	9260(8)	4177(6)	2946(5)	22(3)
C(19)	9161(8)	5050(7)	3142(5)	24(3)
C(20)	9045(9)	5652(7)	2673(5)	29(3)
C(21)	9059(8)	5375(8)	2044(6)	31(3)
C(22)	9148(9)	4494(7)	1846(5)	25(3)
C(23)	8049(10)	4369(7)	854(5)	40(3)
C(24)	10185(9)	4458(7)	831(5)	33(3)
C(25)	10486(9)	2587(6)	1530(5)	22(3)

C(26)	11558(10)	2972(7)	1759(6)	30(3)
C(27)	12556(10)	2940(8)	1395(6)	37(3)
C(28)	12505(10)	2507(7)	793(5)	32(3)
C(29)	11475(10)	2139(8)	561(6)	35(3)
C(30)	10464(10)	2167(7)	914(5)	28(3)
C(31)	9296(12)	821(7)	662(6)	56(4)
C(32)	9042(10)	2072(8)	48(6)	42(3)
C(33)	14891(9)	1242(6)	-2212(5)	19(3)
C(34)	14804(8)	834(7)	-2823(5)	25(3)
C(35)	14685(9)	-75(7)	-2931(6)	28(3)
C(36)	14687(9)	-585(7)	-2413(6)	30(3)
C(37)	14785(9)	-199(6)	-1802(6)	30(3)
C(38)	14906(9)	719(6)	-1707(5)	24(3)
C(39)	14022(10)	918(7)	-669(5)	31(3)
C(40)	16117(9)	986(7)	-762(5)	30(3)
C(41)	16310(9)	2722(6)	-1703(5)	18(2)
C(42)	17288(9)	2306(7)	-1953(6)	31(3)
C(43)	18396(9)	2569(7)	-1726(6)	29(3)
C(44)	18531(10)	3232(7)	-1235(5)	29(3)
C(45)	17573(9)	3645(6)	-990(6)	28(3)
C(46)	16436(9)	3400(7)	-1228(5)	25(3)
C(47)	15160(9)	3499(7)	-345(5)	35(3)
C(48)	15556(9)	4779(7)	-942(5)	35(3)
C(49)	15045(9)	4176(6)	-2724(5)	21(3)
C(50)	14029(10)	4517(7)	-2456(5)	28(3)
C(51)	13942(9)	5413(7)	-2338(5)	29(3)
C(52)	14885(10)	5980(7)	-2481(5)	34(3)
C(53)	15882(10)	5665(7)	-2714(6)	34(3)
C(54)	15990(9)	4748(6)	-2844(5)	21(3)
C(55)	17926(9)	4363(7)	-2613(6)	37(3)
C(56)	17533(11)	4863(8)	-3639(6)	53(4)
C(57)	13612(9)	2791(7)	-3350(5)	24(3)
C(58)	12708(10)	2252(6)	-3130(6)	32(3)
C(59)	11657(10)	2166(7)	-3457(5)	29(3)
C(60)	11527(10)	2581(7)	-4015(6)	36(3)
C(61)	12413(10)	3091(7)	-4240(6)	39(3)
C(62)	13469(10)	3201(7)	-3906(5)	31(3)
C(63)	14147(11)	4655(7)	-4192(6)	50(4)
C(64)	15016(10)	3366(8)	-4672(5)	46(4)

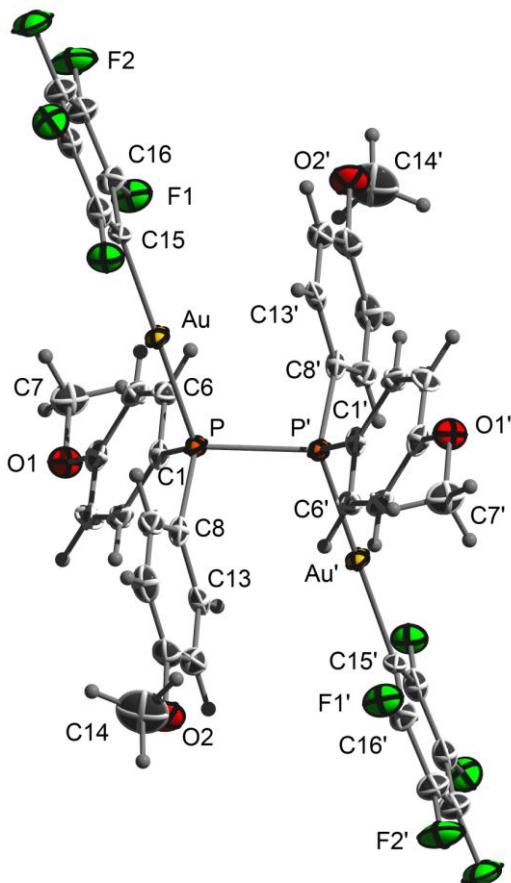
**Table S17.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for compound **2e**. The anisotropic displacement factor exponent takes the form:  $-2p^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^{*} b^{*} U^{12} ]$ .

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
Au(1)	31(1)	26(1)	31(1)	5(1)	-7(1)	-7(1)
Au(2)	23(1)	23(1)	26(1)	2(1)	-2(1)	-3(1)
Au(3)	20(1)	23(1)	25(1)	2(1)	1(1)	0(1)
Au(4)	24(1)	29(1)	28(1)	0(1)	3(1)	-1(1)

Cl(1)	41(2)	52(2)	56(3)	18(2)	-26(2)	-22(2)
Cl(2)	29(2)	36(2)	41(2)	8(2)	-12(2)	-8(1)
Cl(3)	22(2)	35(2)	40(2)	10(2)	8(1)	9(1)
Cl(4)	37(2)	58(2)	46(2)	1(2)	15(2)	12(2)
P(1)	29(2)	19(2)	24(2)	3(1)	1(2)	-2(1)
P(2)	22(2)	22(2)	25(2)	-1(1)	0(1)	-4(1)
P(3)	22(2)	20(2)	24(2)	2(1)	-1(1)	-1(1)
P(4)	22(2)	22(2)	25(2)	2(1)	-1(1)	-3(1)
N(1)	45(7)	28(6)	27(6)	9(5)	-3(5)	2(5)
N(2)	36(6)	25(5)	39(7)	-5(5)	-13(5)	-1(5)
N(3)	24(6)	35(6)	33(7)	5(5)	5(5)	-7(5)
N(4)	30(6)	33(6)	23(6)	-3(5)	-2(5)	-10(5)
N(5)	26(5)	27(5)	19(6)	7(4)	-1(4)	2(4)
N(6)	24(5)	19(5)	20(6)	-11(4)	-2(4)	-7(4)
N(7)	30(6)	19(5)	27(6)	-5(4)	11(5)	6(4)
N(8)	38(6)	39(6)	27(6)	7(5)	3(5)	-12(5)
C(1)	29(7)	11(5)	24(7)	-8(5)	7(5)	-4(5)
C(2)	31(5)	26(4)	30(6)	8(4)	8(4)	-9(4)
C(3)	31(5)	26(4)	30(6)	8(4)	8(4)	-9(4)
C(4)	50(9)	30(7)	51(9)	-5(7)	35(7)	0(7)
C(5)	61(9)	23(7)	34(8)	5(6)	9(7)	-3(7)
C(6)	46(8)	10(6)	32(8)	3(5)	14(6)	-2(6)
C(7)	49(9)	27(7)	50(9)	7(6)	-6(7)	1(6)
C(8)	54(9)	58(9)	23(8)	13(7)	-11(7)	-21(7)
C(9)	30(7)	19(6)	24(7)	4(5)	8(6)	-1(5)
C(10)	21(6)	37(7)	24(7)	6(6)	1(5)	3(6)
C(11)	28(7)	28(7)	34(8)	2(6)	-11(6)	-14(6)
C(12)	44(9)	35(8)	60(10)	0(7)	-4(8)	1(7)
C(13)	25(7)	27(7)	83(12)	-15(7)	-1(7)	10(6)
C(14)	25(7)	29(7)	40(8)	-5(6)	5(6)	-3(6)
C(15)	42(8)	53(9)	38(9)	-3(7)	-4(7)	-20(7)
C(16)	41(8)	50(9)	54(10)	0(7)	8(7)	7(7)
C(17)	22(6)	14(6)	28(7)	-3(5)	-2(5)	-9(5)
C(18)	19(6)	21(6)	26(7)	-3(5)	1(5)	4(5)
C(19)	19(6)	29(6)	25(7)	-4(5)	1(5)	3(5)
C(20)	24(7)	32(7)	30(8)	-1(6)	-4(6)	1(6)
C(21)	11(6)	49(8)	36(8)	20(7)	8(6)	4(6)
C(22)	18(6)	29(7)	28(7)	-4(6)	0(5)	-3(5)
C(23)	45(8)	51(8)	24(8)	11(6)	-11(6)	-6(7)
C(24)	46(8)	36(7)	16(7)	11(6)	6(6)	-3(6)
C(25)	22(6)	21(6)	21(7)	-1(5)	11(5)	3(5)
C(26)	36(7)	22(6)	30(8)	-2(6)	-4(6)	0(6)
C(27)	32(7)	51(8)	29(8)	6(7)	-3(6)	1(7)
C(28)	42(8)	28(7)	25(8)	2(6)	13(6)	-5(6)
C(29)	34(8)	46(8)	25(8)	1(6)	10(6)	-1(6)
C(30)	35(7)	25(6)	22(7)	0(5)	-4(6)	-14(6)
C(31)	82(11)	27(7)	55(10)	-14(7)	-2(9)	-22(7)
C(32)	30(7)	56(9)	37(9)	-11(7)	-7(6)	-6(7)
C(33)	20(6)	11(5)	26(7)	-1(5)	-3(5)	4(5)
C(34)	16(6)	22(6)	37(8)	-1(6)	1(6)	-6(5)

C(35)	23(6)	28(7)	34(8)	-5(6)	-5(6)	7(6)
C(36)	14(6)	26(6)	48(9)	-7(6)	-9(6)	-4(5)
C(37)	23(7)	17(6)	50(9)	4(6)	-1(6)	-1(5)
C(38)	18(6)	20(6)	37(8)	-2(6)	6(6)	9(5)
C(39)	51(8)	24(6)	19(7)	5(5)	1(6)	-4(6)
C(40)	37(7)	29(7)	24(7)	0(5)	-4(6)	-3(6)
C(41)	22(6)	21(6)	11(6)	6(5)	-8(5)	-11(5)
C(42)	29(7)	16(6)	47(9)	-6(6)	4(6)	0(5)
C(43)	22(7)	25(6)	41(8)	8(6)	-1(6)	-2(5)
C(44)	32(7)	25(6)	31(8)	15(6)	-2(6)	-4(6)
C(45)	31(7)	11(6)	43(8)	-1(5)	-5(6)	2(5)
C(46)	21(6)	22(6)	33(8)	5(5)	0(6)	-4(5)
C(47)	32(7)	42(7)	29(8)	-9(6)	5(6)	-6(6)
C(48)	28(7)	41(7)	35(8)	-6(6)	8(6)	3(6)
C(49)	14(6)	24(6)	25(7)	1(5)	-6(5)	4(5)
C(50)	35(7)	27(6)	24(7)	11(5)	-3(6)	-4(6)
C(51)	25(7)	35(7)	29(8)	5(6)	5(6)	5(6)
C(52)	37(8)	33(7)	30(8)	4(6)	-2(6)	-8(6)
C(53)	36(8)	17(6)	49(9)	10(6)	1(7)	-12(6)
C(54)	23(6)	11(5)	30(7)	1(5)	-9(5)	-1(5)
C(55)	18(6)	39(7)	53(9)	1(7)	-2(6)	1(6)
C(56)	47(9)	68(10)	46(10)	16(8)	12(7)	5(8)
C(57)	15(6)	23(6)	34(8)	1(5)	12(5)	4(5)
C(58)	40(8)	19(6)	35(8)	3(6)	3(6)	-1(6)
C(59)	24(7)	32(7)	31(8)	6(6)	1(6)	-2(6)
C(60)	37(8)	38(7)	30(8)	-8(6)	4(6)	-11(6)
C(61)	42(8)	47(8)	27(8)	4(6)	-13(7)	-7(7)
C(62)	42(8)	29(7)	20(7)	1(6)	-4(6)	-5(6)
C(63)	46(9)	43(8)	64(11)	26(8)	4(8)	-7(7)
C(64)	39(8)	77(10)	18(8)	-4(7)	-10(6)	-14(7)

## 2.8 Crystal Structure Determination of **2h**



**Figure S14.** ORTEP Plot of compound **2h**. Ellipsoids are drawn at the 50% probability level.

**Table S18.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for compound **2h**. U(eq) is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	U(eq)
Au(1)	1524(1)	9718(1)	3174(1)	16(1)
P(1)	3435(2)	9784(1)	4894(1)	14(1)
F(1)	668(4)	7281(3)	947(2)	32(1)
O(1)	2248(5)	4525(3)	4905(3)	25(1)
C(1)	3179(6)	8202(4)	4953(4)	14(1)
F(2)	-1725(5)	6601(3)	-1192(2)	43(1)
O(2)	3139(5)	14003(3)	9050(3)	34(1)
C(2)	2760(6)	7965(4)	5856(4)	18(1)
F(3)	-3837(4)	8309(3)	-1801(2)	42(1)
C(3)	2445(6)	6727(4)	5805(4)	21(1)
F(4)	-3514(4)	10698(3)	-238(2)	33(1)
C(4)	2552(6)	5706(4)	4863(4)	18(1)
F(5)	-1196(4)	11373(2)	1916(2)	28(1)
C(5)	2959(6)	5921(4)	3955(4)	20(1)

C(6)	3248(6)	7173(4)	4006(4)	18(1)
C(7)	2283(8)	3455(4)	3924(4)	30(1)
C(8)	3204(6)	10974(4)	6191(4)	14(1)
C(9)	2032(6)	11870(4)	6039(4)	20(1)
C(10)	1966(6)	12906(4)	6980(4)	24(1)
C(11)	3052(7)	13037(4)	8066(4)	23(1)
C(12)	4214(6)	12121(4)	8214(4)	22(1)
C(13)	4268(6)	11097(4)	7274(4)	16(1)
C(14)	2075(10)	15007(5)	8962(6)	53(2)
C(15)	-190(6)	9356(5)	1533(4)	21(1)
C(16)	-373(6)	8162(4)	689(4)	21(1)
C(17)	-1582(7)	7778(5)	-423(4)	28(1)
C(18)	-2659(7)	8631(5)	-730(4)	28(1)
C(19)	-2483(6)	9851(4)	78(4)	23(1)
C(20)	-1257(6)	10176(4)	1188(4)	23(1)

**Table S19.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for compound **2h**. The anisotropic displacement factor exponent takes the form:  $-2p^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^{*} b^{*} U^{12} ]$ .

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
Au(1)	13(1)	21(1)	14(1)	9(1)	0(1)	1(1)
P(1)	13(1)	15(1)	11(1)	5(1)	1(1)	2(1)
F(1)	37(2)	29(2)	29(2)	10(1)	6(1)	16(1)
O(1)	34(2)	16(2)	25(2)	9(2)	9(2)	2(1)
C(1)	10(1)	15(2)	21(2)	11(1)	3(1)	2(1)
F(2)	56(2)	39(2)	23(2)	0(1)	7(1)	14(2)
O(2)	41(2)	24(2)	29(2)	-3(2)	13(2)	9(2)
C(2)	17(2)	16(2)	15(2)	3(2)	4(2)	3(2)
F(3)	39(2)	53(2)	20(2)	10(2)	-6(1)	6(2)
C(3)	23(2)	25(2)	20(2)	14(2)	7(2)	3(2)
F(4)	29(2)	44(2)	36(2)	27(2)	7(1)	17(1)
C(4)	13(2)	17(2)	23(2)	9(2)	2(2)	1(2)
F(5)	34(2)	24(2)	26(2)	8(1)	9(1)	9(1)
C(5)	20(2)	16(2)	18(2)	4(2)	4(2)	1(2)
C(6)	20(2)	19(2)	14(2)	7(2)	4(2)	0(2)
C(7)	40(3)	16(2)	29(3)	8(2)	8(2)	2(2)
C(8)	10(1)	15(2)	21(2)	11(1)	3(1)	2(1)
C(9)	17(2)	24(2)	20(2)	10(2)	4(2)	2(2)
C(10)	20(2)	21(2)	35(3)	13(2)	12(2)	11(2)
C(11)	24(2)	18(2)	25(3)	1(2)	12(2)	2(2)
C(12)	21(2)	23(2)	20(2)	6(2)	6(2)	0(2)
C(13)	15(2)	15(2)	21(2)	6(2)	11(2)	2(2)
C(14)	73(5)	28(3)	55(4)	2(3)	29(4)	25(3)
C(15)	15(2)	36(3)	12(2)	11(2)	3(2)	-2(2)
C(16)	18(2)	24(2)	21(2)	10(2)	4(2)	8(2)
C(17)	25(2)	37(2)	20(2)	10(2)	2(1)	3(2)
C(18)	25(2)	37(2)	20(2)	10(2)	2(1)	3(2)
C(19)	19(2)	24(2)	29(2)	10(2)	12(1)	4(1)
C(20)	19(2)	24(2)	29(2)	10(2)	12(1)	4(1)

### 3. References

- 
- [1] G. M. Sheldrick, *Acta Cryst.* **2008**, *A64*, 112–122.
  - [2] A. L. Spek, *J. Appl. Cryst.* 2003, **36**, 7-13.