Electronic Supplementary Material (ESI) for Dalton Transactions
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Supporting information

Zn(II) Robson macrocycles as templates for chelating diphosphines

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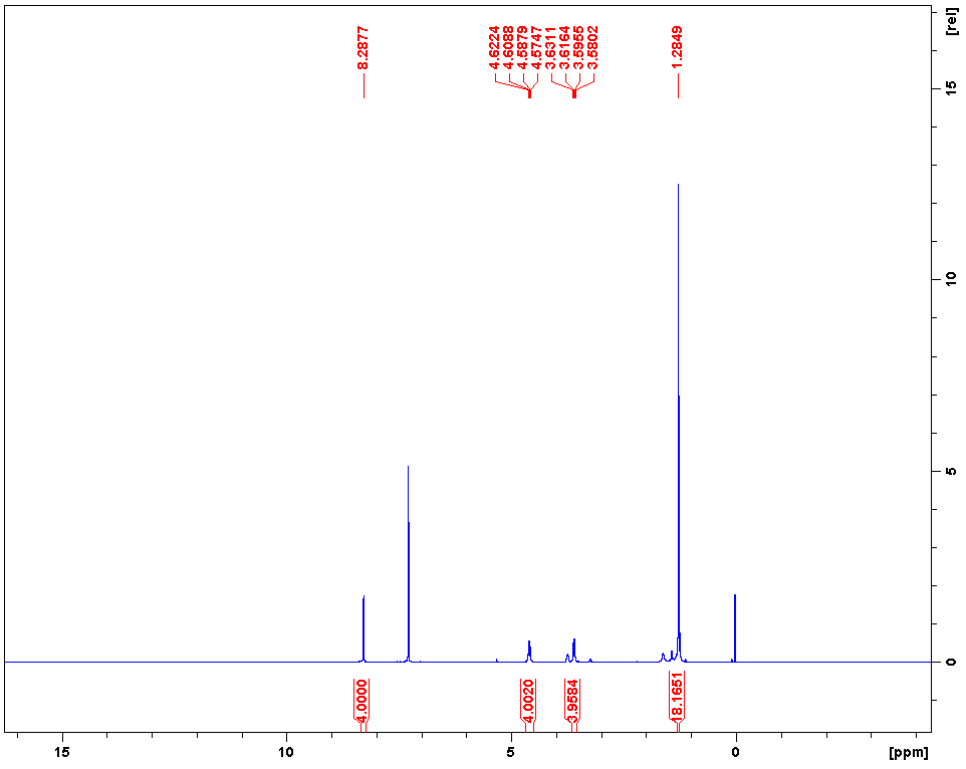
Robson macrocycles

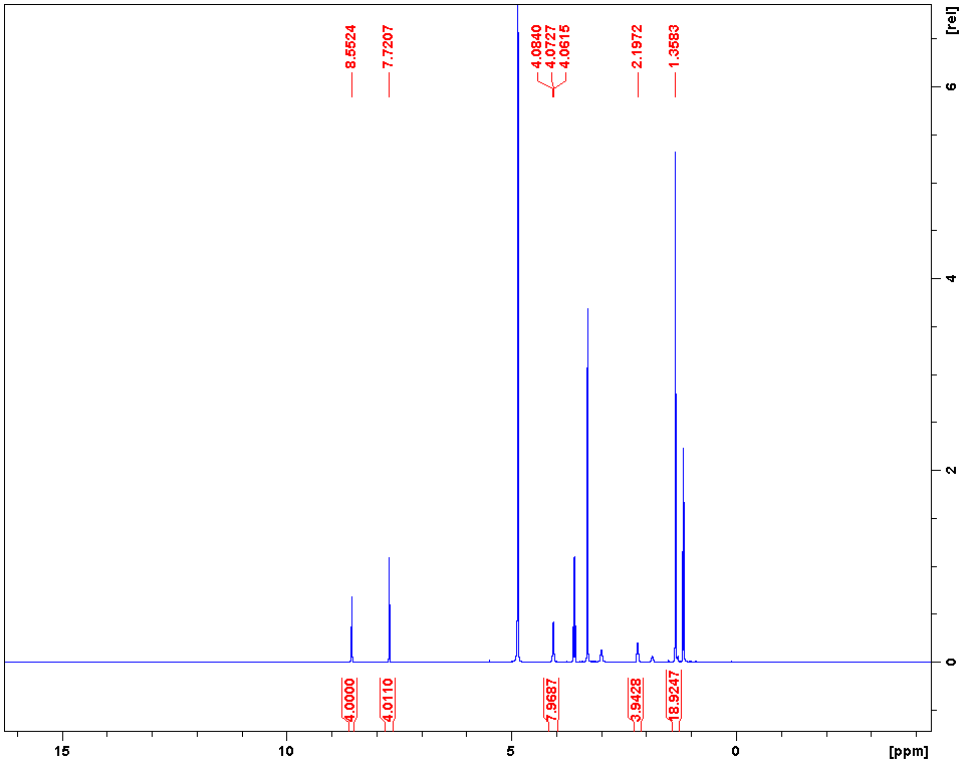
2

^{1}H-NMR (400 MHz, chlrorform-d_1)

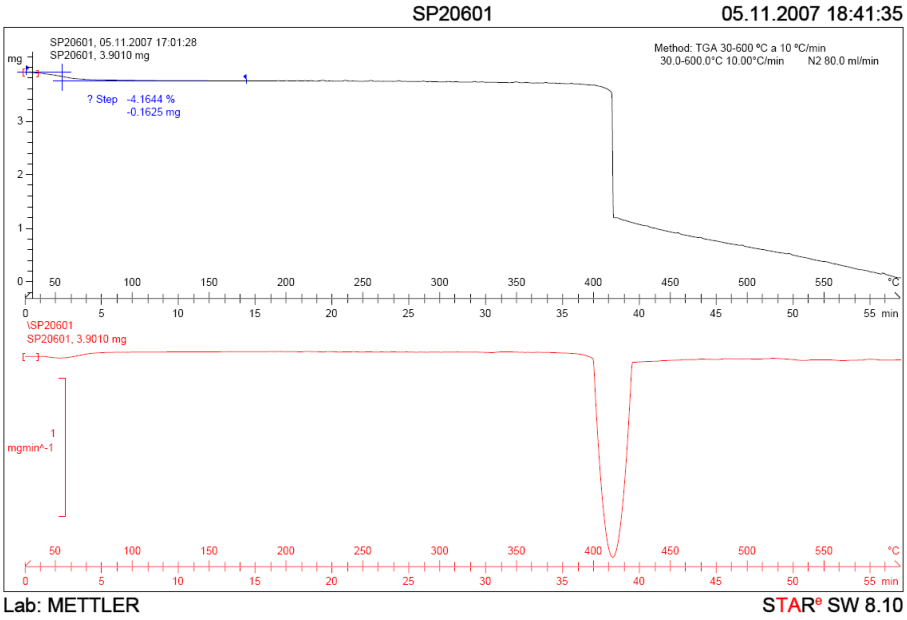


3

^{1}H-NMR (400 MHz, methanol-d_4)



Thermo-Gravimetric Analysis



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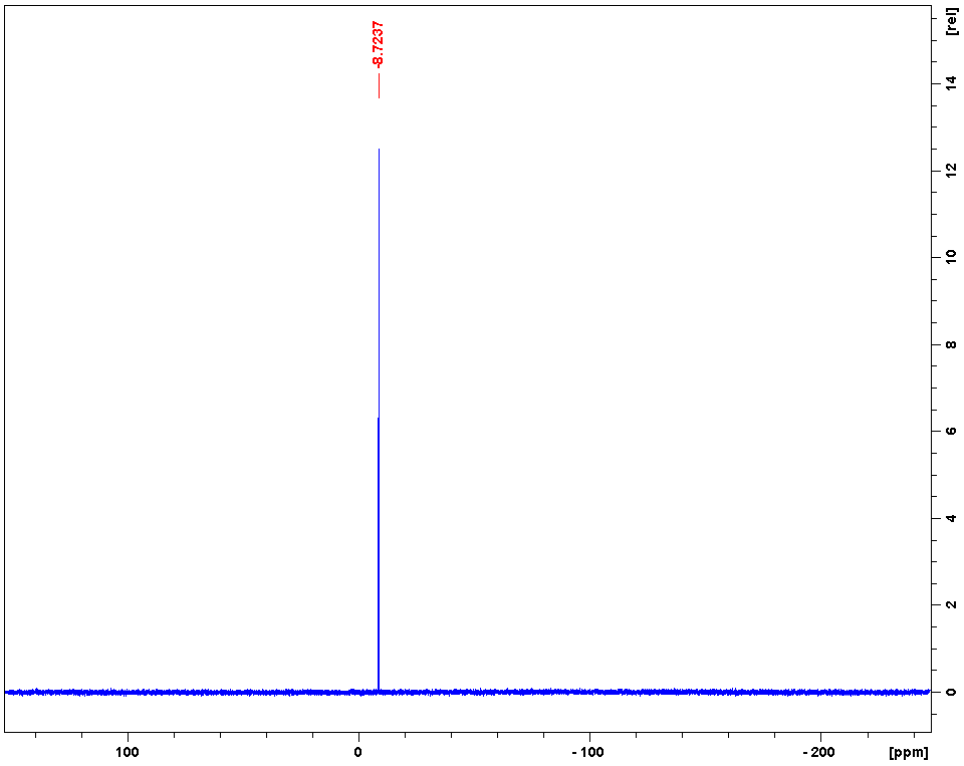
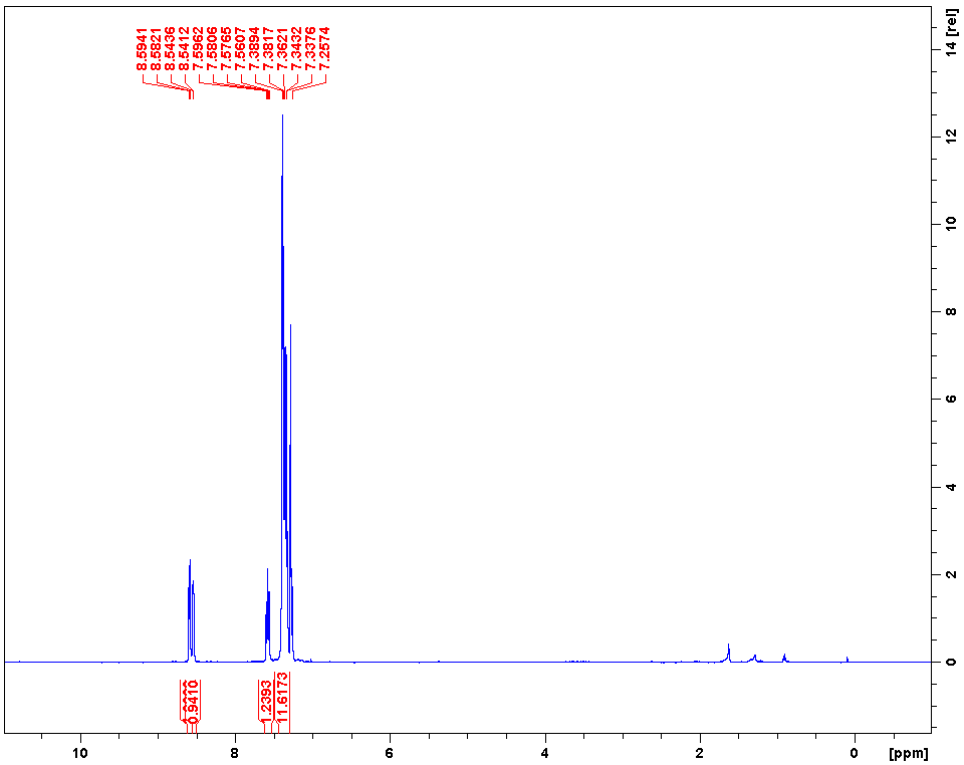
Ditopic ligands

3-(diphenylphosphino)pyridine. (A)

^{31}P-{^{1}H}-NMR (161 MHz, chloroform-d_1)



^{1}H-NMR (400 MHz, chloroform-d_1)



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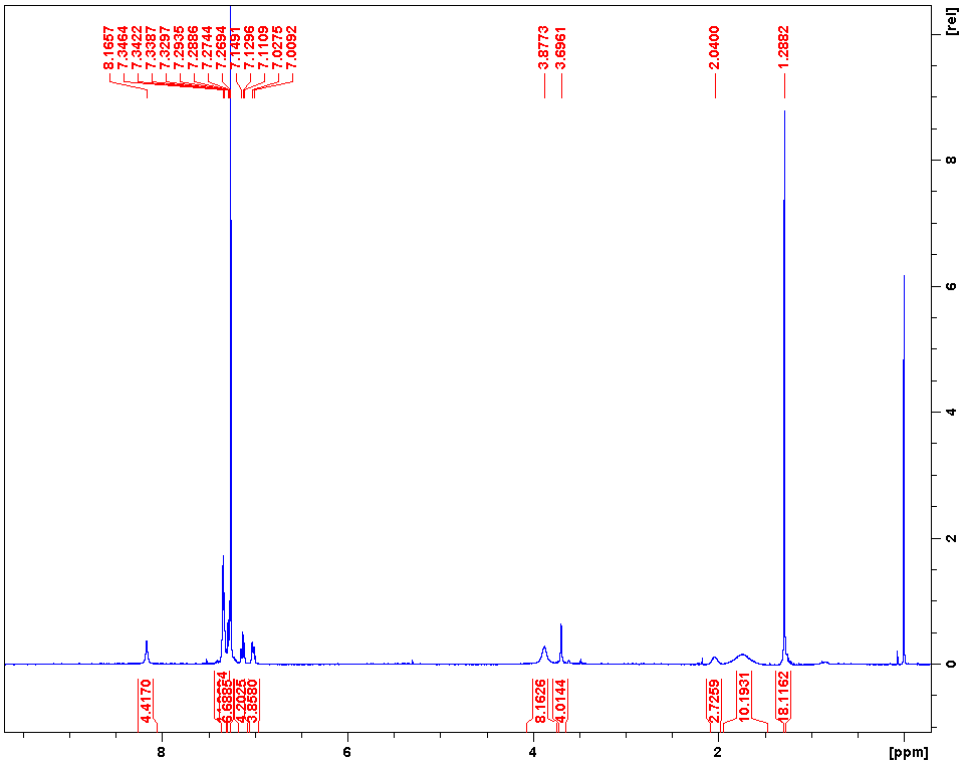
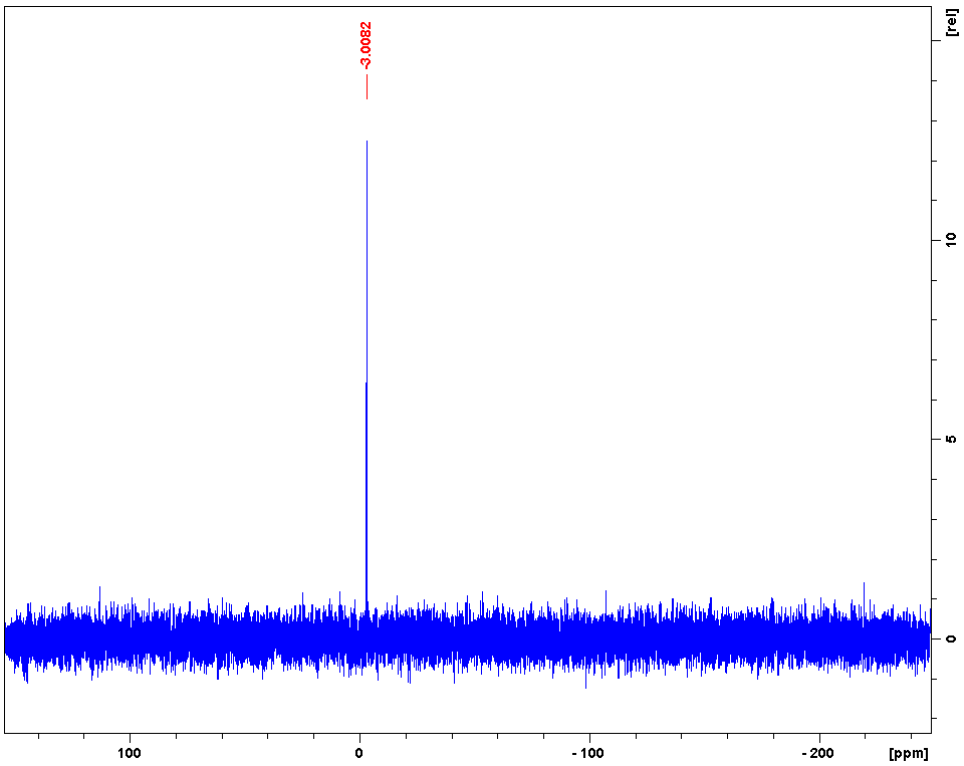
Self assembled diphosphines

7C

^{1}H-NMR (400 MHz, chloroform-d_1)



^{31}P-{^{1}H}-NMR (161 MHz, chloroform-d_1)



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Single Crystal X-Ray Diffraction Data 7C

Table 1. Crystal data and structure refinement for SP218_0m.

Identification code	SP218_0m	
Empirical formula	C70 H76 Cl8 N6 O10 P2 Zn2	
Formula weight	1637.65	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 8.8886(14) Å	α= 90.00 °
	b = 21.225(4) Å	β = 90.878(8) °
	c = 19.390(3) Å	γ = 90.00 °
Volume	3657.7(10) Å^3	
Z	2	
Density (calculated)	1.487 Mg/m^3	
Absorption coefficient	1.053 mm^{-1}	
F(000)	1688	
Crystal size	0.05 x 0.02 x 0.005 mm^3	
Theta range for data collection	2.48 to 25.64 °.	
Index ranges	$-9 \le h \le 10$, $-25 \le k \le 25$, $-19 \le l \le 23$	
Reflections collected	6814	
Independent reflections	2641 [R_{int} = 0.2768]	
Completeness to theta =25.64 °	0.987 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9948 and 0.9492	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6814 / 54 / 482	
Goodness-of-fit on F_2	0.933	
Final R indices [I>2sigma(I)]	R_1 = 0.0915 , wR_2 = 0.1844	
R indices (all data)	R_1 = 0.2536 , wR_2 = 0.2497	
Largest diff. peak and hole	1.537 and -0.907 e·Å^{-3}	

Table 2. Bond lengths [Å] and angles [°] for SP218_0m.

Bond lengths				Angles					
C1-O1	1.337(8)	N2-C35#1	1.288(9)	O1-C1-C2	120.5(7)	C24-C29-C28	120.0(8)	O2S'-Cl1S-O4S	113.8(5)
C1-C2	1.409(11)	N2-Zn1	2.056(6)	O1-C1-C6	121.6(7)	N1-C31-C32	110.7(7)	C18-P1-C12	104.0(4)
C1-C6	1.413(10)	N3-Zn1	2.077(6)	C2-C1-C6	117.9(7)	C31-C32-C33	115.1(7)	C18-P1-C24	104.2(4)
C2-C3	1.408(11)	O1-Zn1#1	2.008(5)	C3-C2-C1	120.2(7)	N2-C33-C32	112.6(6)	C12-P1-C24	100.5(3)
C2-C11	1.457(11)	O1-Zn1	2.110(5)	C3-C2-C11	114.9(7)	N3-C34-C15	109.9(7)	O1-Zn1-N1#1	144.9(2)
C3-C4	1.371(11)	Cl1S-O2S	1.334(9)	C1-C2-C11	124.6(7)	N2-C35-C6#1	128.6(7)	O1-Zn1-N2#1	90.0(2)
C4-C5	1.400(11)	Cl1S-O4S'	1.343(9)	C4-C3-C2	123.3(8)	Cl1A-C1A-Cl3A	111.5(5)	N1-Zn1-N2	94.4(3)
C4-C7	1.521(11)	Cl1S-O1S	1.391(8)	C3-C4-C5	115.5(7)	Cl1A-C1A-Cl2A	110.4(5)	O1-Zn1-N3#1	102.6(2)
C5-C6	1.405(10)	Cl1S-O3S	1.463(8)	C3-C4-C7	123.6(8)	Cl3A-C1A-Cl2A	110.4(5)	N1-Zn1-N3	107.1(3)
C6-C35	1.435(11)	Cl1S-O3S'	1.463(9)	C5-C4-C7	120.7(7)	C11-N1-C31	115.6(7)	N2-Zn1-N3	114.2(3)
C7-C10	1.494(12)	Cl1S-O1S'	1.474(8)	C4-C5-C6	124.1(7)	C11-N1-Zn1	124.9(6)	O1-Zn1-O1#1	75.3(2)
C7-C8	1.536(12)	Cl1S-O2S'	1.479(7)	C5-C6-C1	118.8(7)	C31-N1-Zn1	119.1(5)	N1-Zn1-O1	85.8(2)
C7-C9	1.578(12)	Cl1S-O4S	1.577(9)	C5-C6-C35	116.6(7)	C35-N2-C33#1	113.4(6)	N2-Zn1-O1	153.1(2)
C11-N1	1.283(10)	Zn1-O1#1	2.008(5)	C1-C6-C35	124.5(7)	C35-N2-Zn1#1	123.6(5)	N3-Zn1-O1	91.3(2)
C12-C17	1.395(10)			C10-C7-C4	113.6(7)	C33-N2-Zn1	123.0(5)		
C12-C13	1.406(11)			C10-C7-C8	110.7(7)	C34-N3-Zn1	121.5(4)		
C12-P1	1.829(9)			C4-C7-C8	110.1(7)	C1-O1-Zn1#1	128.2(4)		
C13-C14	1.374(11)			C10-C7-C9	106.6(8)	C1-O1-Zn1	127.0(4)		
C14-C15	1.392(10)			C4-C7-C9	109.1(6)	Zn1-O1-Zn1#1	104.7(2)		
C15-C16	1.388(11)			C8-C7-C9	106.6(7)	O2S-Cl1S-O4S'	96.1(8)		
C15-C34	1.523(11)			N1-C11-C2	127.6(7)	O2S-Cl1S-O1S	120.9(7)		
C16-C17	1.370(12)			C17-C12-C13	117.4(8)	O4S'-Cl1S-O1S	123.4(7)		
C18-C19	1.350(13)			C17-C12-P1	117.6(6)	O2S-Cl1S-O3S	110.5(6)		
C18-C23	1.408(12)			C13-C12-P1	125.0(6)	O4S'-Cl1S-O3S	92.5(7)		
C18-P1	1.811(9)			C14-C13-C12	121.4(7)	O1S-Cl1S-O3S	109.6(5)		
C19-C20	1.362(13)			C13-C14-C15	120.0(7)	O2S-Cl1S-O3S'	93.2(7)		
C20-C21	1.363(13)			C16-C15-C14	118.9(7)	O4S'-Cl1S-O3S'	117.5(7)		
C21-C22	1.348(14)			C16-C15-C34	122.2(7)	O1S-Cl1S-O3S'	102.6(7)		
C22-C23	1.414(13)			C14-C15-C34	118.8(7)	O3S-Cl1S-O3S'	28.4(5)		
C24-C25	1.376(11)			C17-C16-C15	120.8(7)	O2S-Cl1S-O1S'	132.3(7)		
C24-C29	1.384(11)			C16-C17-C12	121.1(8)	O4S'-Cl1S-O1S'	112.2(6)		
C24-P1	1.834(7)			C19-C18-C23	117.8(9)	O1S-Cl1S-O1S'	12.9(6)		
C25-C26	1.387(11)			C19-C18-P1	126.2(7)	O3S-Cl1S-O1S'	105.9(6)		
C26-C27	1.366(13)			C23-C18-P1	116.0(7)	O3S'-Cl1S-O1S'	105.4(5)		
C27-C28	1.386(13)			C18-C19-C20	123.3(9)	O2S-Cl1S-O2S'	26.0(6)		
C28-C29	1.409(10)			C19-C20-C21	120.1(10)	O4S'-Cl1S-O2S'	111.6(5)		
C31-N1	1.477(10)			C22-C21-C20	118.9(10)	O1S-Cl1S-O2S'	95.1(6)		
C31-C32	1.505(12)			C21-C22-C23	122.0(9)	O3S-Cl1S-O2S'	127.6(6)		
C32-C33	1.506(11)			C18-C23-C22	117.9(10)	O3S'-Cl1S-O2S'	102.7(6)		
C33-N2	1.472(10)			C25-C24-C29	119.1(7)	O1S'-Cl1S-O2S'	106.4(5)		
C34-N3	1.491(11)			C25-C24-P1	117.2(6)	O2S-Cl1S-O4S	106.2(6)		
C35-N2#1	1.288(9)			C29-C24-P1	123.7(6)	O4S'-Cl1S-O4S	20.1(6)		
C1A-Cl1A	1.740(9)			C24-C25-C26	121.4(8)	O1S-Cl1S-O4S	103.7(6)		
C1A-Cl3A	1.753(10)			C27-C26-C25	119.6(9)	O3S-Cl1S-O4S	104.4(6)		
C1A-Cl2A	1.764(9)			C26-C27-C28	120.6(8)	O3S'-Cl1S-O4S	132.2(7)		
N1-Zn1	2.052(7)			C27-C28-C29	119.3(8)	O1S'-Cl1S-O4S	93.1(7)		

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

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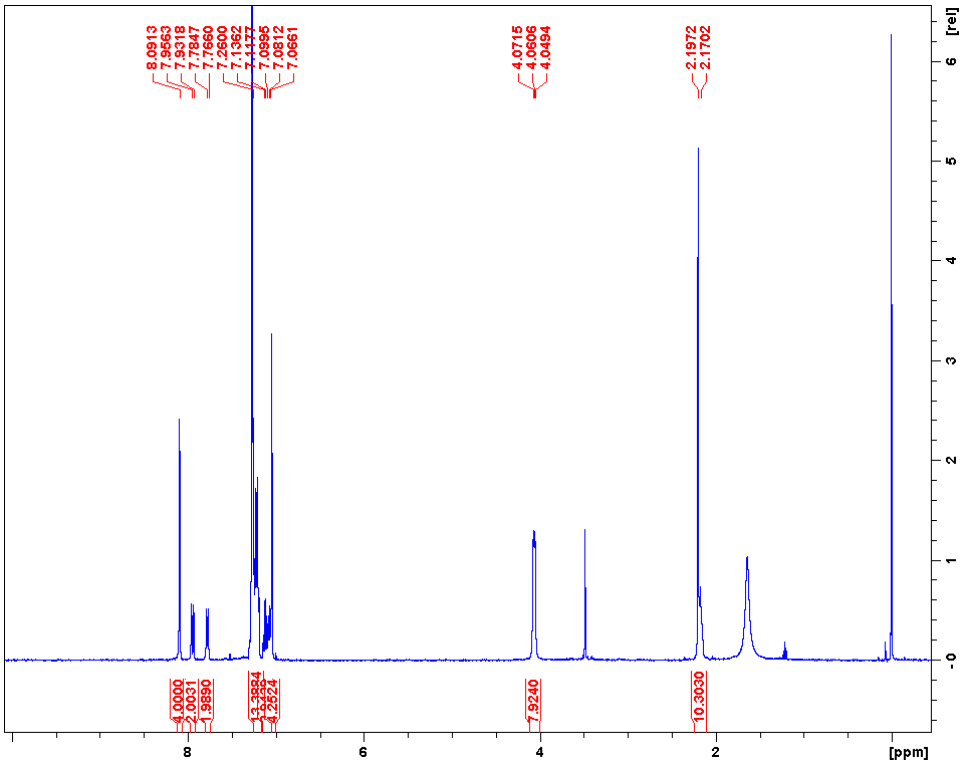
Table 3. Torsion angles [°] for SP218_0m.

O1-C1-C2-C3	-177.5(7)	C13-C14-C15-C16	6.4(12)	C5-C6-C35-N2#1	-165.7(8)	C11-N1-Zn1-N2	179.9(6)
C6-C1-C2-C3	3.9(10)	C13-C14-C15-C34	-178.6(8)	C1-C6-C35-N2#1	10.1(13)	C31-N1-Zn1-N2	8.1(6)
O1-C1-C2-C11	-3.4(11)	C14-C15-C16-C17	-8.1(13)	C2-C11-N1-C31	-173.8(7)	C11-N1-Zn1-N3	62.9(7)
C6-C1-C2-C11	177.9(7)	C34-C15-C16-C17	177.1(8)	C2-C11-N1-Zn1	14.1(11)	C31-N1-Zn1-N3	-108.9(6)
C1-C2-C3-C4	-2.6(12)	C15-C16-C17-C12	4.4(13)	C32-C31-N1-C11	-136.4(7)	C11-N1-Zn1-O1	-27.1(6)
C11-C2-C3-C4	-177.2(7)	C13-C12-C17-C16	1.0(13)	C32-C31-N1-Zn1	36.1(8)	C31-N1-Zn1-O1	161.1(6)
C2-C3-C4-C5	-1.1(11)	P1-C12-C17-C16	-179.0(7)	C32-C33-N2-C35#1	-179.7(7)	C35#1-N2-Zn1-O1#1	6.2(6)
C2-C3-C4-C7	174.2(7)	C23-C18-C19-C20	-0.5(11)	C32-C33-N2-Zn1	-1.3(9)	C33-N2-Zn1-O1#1	-172.0(6)
C3-C4-C5-C6	3.5(11)	P1-C18-C19-C20	176.2(6)	C15-C34-N3-Zn1	-57.4(7)	C35#1-N2-Zn1-N1	151.4(6)
C7-C4-C5-C6	-171.9(7)	C18-C19-C20-C21	0.5(12)	C2-C1-O1-Zn1#1	160.6(5)	C33-N2-Zn1-N1	-26.9(6)
C4-C5-C6-C1	-2.1(11)	C19-C20-C21-C22	0.3(12)	C6-C1-O1-Zn1#1	-20.9(9)	C35#1-N2-Zn1-N3	-97.7(6)
C4-C5-C6-C35	173.9(7)	C20-C21-C22-C23	-0.9(13)	C2-C1-O1-Zn1	-23.4(9)	C33-N2-Zn1-N3	84.1(6)
O1-C1-C6-C5	179.7(6)	C19-C18-C23-C22	-0.1(11)	C6-C1-O1-Zn1	155.2(5)	C35#1-N2-Zn1-O1	62.0(9)
C2-C1-C6-C5	-1.7(10)	P1-C18-C23-C22	-177.2(6)	C19-C18-P1-C12	-23.4(7)	C33-N2-Zn1-O1	-116.2(6)
O1-C1-C6-C35	4.1(11)	C21-C22-C23-C18	0.9(12)	C23-C18-P1-C12	153.3(6)	C34-N3-Zn1-O1#1	-51.2(6)
C2-C1-C6-C35	-177.4(7)	C29-C24-C25-C26	-1.0(13)	C19-C18-P1-C24	81.5(7)	C34-N3-Zn1-N1	147.6(5)
C3-C4-C7-C10	-0.3(11)	P1-C24-C25-C26	179.2(7)	C23-C18-P1-C24	-101.8(6)	C34-N3-Zn1-N2	44.6(6)
C5-C4-C7-C10	174.7(7)	C24-C25-C26-C27	0.6(14)	C17-C12-P1-C18	-101.9(7)	C34-N3-Zn1-O1	-126.4(6)
C3-C4-C7-C8	124.5(8)	C25-C26-C27-C28	-0.2(14)	C13-C12-P1-C18	78.1(8)	C1-O1-Zn1-O1#1	-176.8(7)
C5-C4-C7-C8	-60.5(10)	C26-C27-C28-C29	0.3(14)	C17-C12-P1-C24	150.4(7)	Zn1#1-O1-Zn1-O1#1	0.0
C3-C4-C7-C9	-118.9(9)	C25-C24-C29-C28	1.1(12)	C13-C12-P1-C24	-29.5(8)	C1-O1-Zn1-N1	33.0(6)
C5-C4-C7-C9	56.1(10)	P1-C24-C29-C28	-179.2(6)	C25-C24-P1-C18	177.0(7)	Zn1#1-O1-Zn1-N1	-150.2(3)
C3-C2-C11-N1	-177.0(8)	C27-C28-C29-C24	-0.7(13)	C29-C24-P1-C18	-2.8(8)	C1-O1-Zn1-N2	124.4(6)
C1-C2-C11-N1	8.7(13)	N1-C31-C32-C33	-81.0(9)	C25-C24-P1-C12	-75.5(7)	Zn1#1-O1-Zn1-N2	-58.8(6)
C17-C12-C13-C14	-2.6(12)	C31-C32-C33-N2	60.0(10)	C29-C24-P1-C12	104.8(8)	C1-O1-Zn1-N3	-74.0(6)
P1-C12-C13-C14	177.3(7)	C16-C15-C34-N3	-66.4(9)	C11-N1-Zn1-O1#1	-83.8(7)	Zn1#1-O1-Zn1-N3	102.8(3)
C12-C13-C14-C15	-1.1(13)	C14-C15-C34-N3	118.7(8)	C31-N1-Zn1-O1#1	104.4(6)		

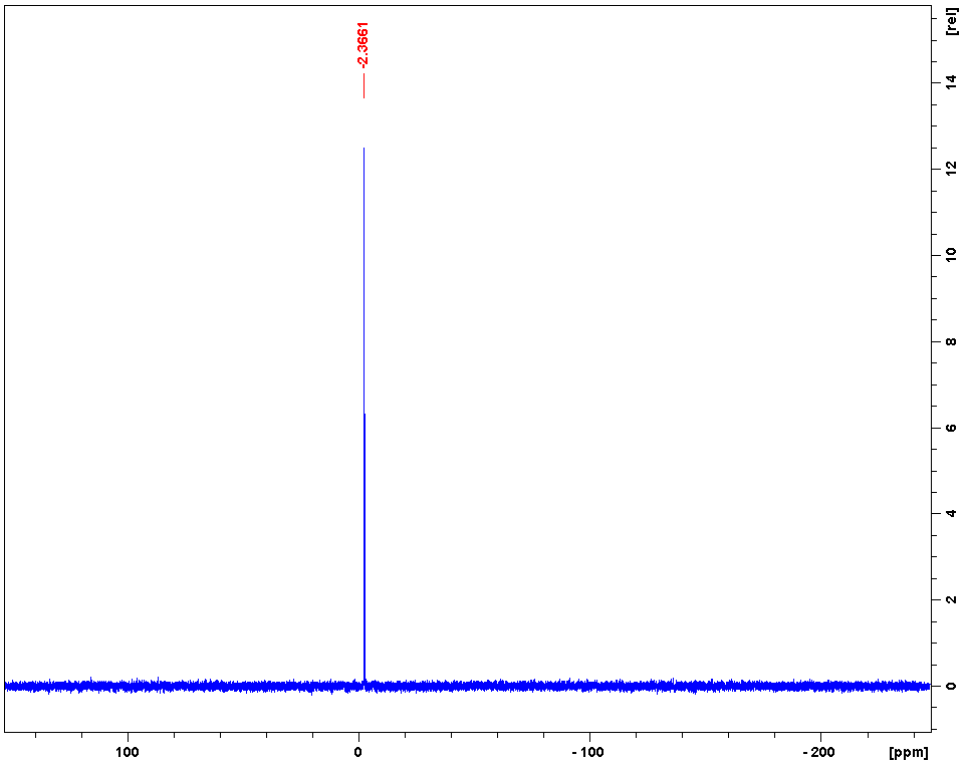
Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y+1, -z+1

9E’

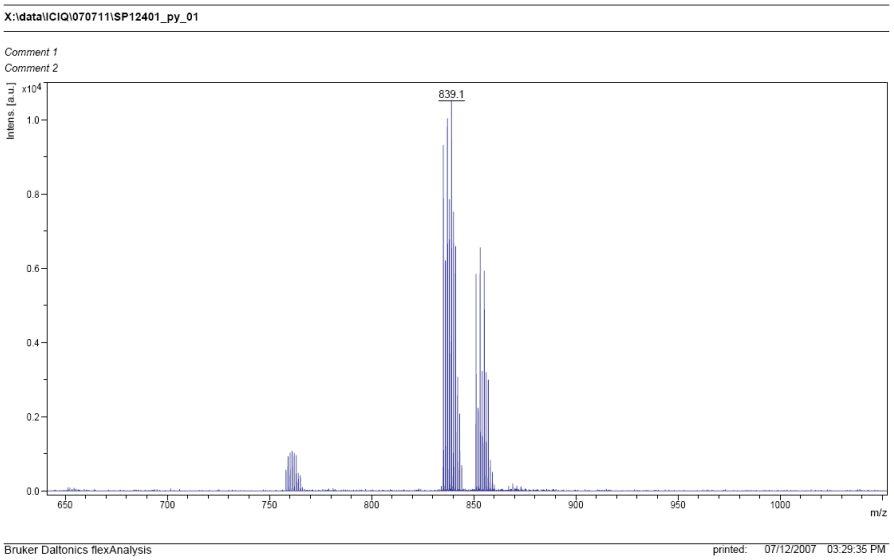
^{1}H-NMR (400 MHz, chloroform-d_1)



^{31}P-{^{1}H}-NMR (161 MHz, chloroform-d_1)



MALDI-TOF-MS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0.0
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750
800
850
900
950
1000
m/z
Bruker Daltonics flexAnalysis
printed: 07/12/2007 03:29:35 PM

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Single Crystal X-Ray Diffraction Data **9E´**

Table 1. Crystal data and structure refinement for SP12401_0m.

Identification code	SP12401_0m	
Empirical formula	C66 H70 N4 O10 P2 Zn2	
Formula weight	1271.94	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 18.8474(12) Å	α= 90.00 °
	b = 7.8500(5) Å	β= 98.266(3) °
	c = 20.6464(13) Å	γ= 90.00 °
Volume	3022.9(3) Å^3	
Z	2	
Density (calculated)	1.397 Mg/m^3	
Absorption coefficient	0.909 mm^{-1}	
F(000)	1328	
Crystal size	0.20 x 0.05 x 0.02 mm^3	
Theta range for data collection	2.74 to 33.96 °.	
Index ranges	$-29 \le h \le 29$, $-8 \le k \le 12$, $-32 \le l \le 32$	
Reflections collected	12184	
Independent reflections	9971 [R_{int} = 0.0454]	
Completeness to theta =33.96 °	0.989 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9820 and 0.8390	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12184 / 559 / 724	
Goodness-of-fit on F_2	1.150	
Final R indices [I>2sigma(I)]	R_1 = 0.0643 , wR_2 = 0.1678	
R indices (all data)	R_1 = 0.0785 , wR_2 = 0.1758	
Largest diff. peak and hole	2.777 and -0.778 e · Å^{-3}	

- SP12401_0m

Compound **9E'** crystallizes in the space group $P2_1/n$, containing half of the molecule in the asymmetric unit. The whole fragment present in the asymmetric unit is disordered over two positions which were refined mutually exclusive leading to 78:22. Atoms of the lowest occupancy part were restrained to have the same bond lengths and angles. In addition, distances of the trimethyl amine fragment were restrained to be consistent. Zn atoms of the two disordered parts were constrained to have the same displacement parameters as well as O1 and N2 atoms. Anisotropic displacement parameters of all atoms were restrained to approximate isotropic behavior.

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Table 2. Bond lengths [Å] and angles [°] for SP12401_0m.

Bond lengths----				Angles----------					
C1-O1	1.316(3)	C1'-C6'	1.418(6)	O1-C1-C2	122.2(3)	C7-N1-Zn1	125.6(2)	C16'-C17'-C18'	119.4(6)
C1-C2	1.418(4)	C1'-C2'	1.419(6)	O1-C1-C6	121.1(3)	C8-N1-Zn1	118.0(3)	C19'-C18'-C17'	118.6(5)
C1-C6	1.420(4)	C2'-C3'	1.414(6)	C2-C1-C6	116.7(3)	C10-N2-C11	114.7(3)	C19'-C18'-P1'	125.4(5)
C2-C3	1.415(4)	C2'-C7'	1.433(6)	C3-C2-C1	120.2(4)	C10-N2-Zn1#1	121.0(2)	C17'-C18'-P1'	115.8(5)
C2-C7	1.431(5)	C3'-C4'	1.368(7)	C3-C2-C7	115.1(3)	C11-N2-Zn1#1	123.6(2)	C18'-C19'-C14'	121.2(6)
C3-C4	1.370(6)	C4'-C5'	1.375(7)	C1-C2-C7	124.7(3)	C1-O1-Zn1#1	125.0(2)	C25'-C20'-C21'	117.4(5)
C4-C5	1.377(6)	C4'-C9'	1.517(6)	C4-C3-C2	123.0(3)	C1-O1-Zn1	130.1(2)	C25'-C20'-P1'	117.3(6)
C4-C9	1.517(4)	C5'-C6'	1.413(5)	C3-C4-C5	116.9(3)	Zn1-O1-Zn1#1	102.78(9)	C21'-C20'-P1'	122.8(5)
C5-C6	1.411(4)	C6'-C10'	1.439(7)	C3-C4-C9	122.9(4)	C13-O2-Zn1	121.8(2)	C22'-C21'-C20'	120.1(6)
C6-C10	1.442(5)	C7'-N1'	1.292(6)	C5-C4-C9	120.1(4)	C20-P1-C18	102.53(14)	C23'-C22'-C21'	119.8(6)
C7-N1	1.294(5)	C8'-N1'	1.474(6)	C4-C5-C6	123.0(3)	C20-P1-C26	101.85(17)	C24'-C23'-C22'	119.3(6)
C8-N1	1.475(4)	C8'-C12'#1	1.693(17)	C5-C6-C1	120.1(4)	C18-P1-C26	103.06(15)	C23'-C24'-C25'	120.3(7)
C8-C12#1	1.505(6)	C10'-N2'	1.292(6)	C5-C6-C10	115.3(3)	O2-Zn1-O1#1	98.74(12)	C24'-C25'-C20'	120.7(6)
C10-N2	1.296(4)	C11'-N2'	1.481(6)	C1-C6-C10	124.6(3)	O2-Zn1-O1	106.54(11)	C31'-C26'-C27'	117.6(6)
C11-N2	1.473(4)	C11'-C12'	1.553(7)	N1-C7-C2	128.3(3)	O1-Zn1-O1#1	77.22(9)	C31'-C26'-P1'	125.1(5)
C11-C12	1.558(6)	C12'-C8'#1	1.693(17)	N1-C8-C12#1	112.0(3)	O2-Zn1-N1	114.53(12)	C27'-C26'-P1'	117.2(5)
C12-C8#1	1.505(6)	C13'-O3'	1.247(6)	N2-C10-C6	128.4(3)	O1-Zn1-N1#1	146.26(13)	C28'-C27'-C26'	121.2(6)
C13-O3	1.248(4)	C13'-O2'	1.271(5)	N2-C11-C12	113.2(3)	O1-Zn1-N1	87.63(10)	C27'-C28'-C29'	120.3(6)
C13-O2	1.272(3)	C13'-C14'	1.518(6)	C8-C12-C11#1	111.6(3)	O2-Zn1-N2#1	98.31(13)	C28'-C29'-C30'	119.0(6)
C13-C14	1.516(4)	C14'-C15'	1.374(6)	O3-C13-O2	124.3(3)	O1#1-Zn1-N2#1	87.90(9)	C29'-C30'-C31'	120.4(6)
C14-C15	1.375(5)	C14'-C19'	1.391(5)	O3-C13-C14	119.9(2)	O1-Zn1-N2#1	152.59(12)	C30'-C31'-C26'	120.9(6)
C14-C19	1.390(4)	C15'-C16'	1.390(6)	O2-C13-C14	115.9(3)	N1-Zn1-N2#1	92.52(11)	C7'-N1'-C8'	118.3(6)
C15-C16	1.389(5)	C16'-C17'	1.386(6)	C15-C14-C19	120.2(3)	O1'-C1'-C6'	122.0(5)	C7'-N1'-Zn1'	124.8(5)
C16-C17	1.385(4)	C17'-C18'	1.409(6)	C15-C14-C13	120.8(2)	O1'-C1'-C2'	121.1(5)	C8'-N1'-Zn1'	116.8(5)
C17-C18	1.408(5)	C18'-C19'	1.390(6)	C19-C14-C13	118.9(3)	C6'-C1'-C2'	116.9(5)	C10'-N2'-C11'	112.9(6)
C18-C19	1.390(4)	C18'-P1'	1.835(4)	C14-C15-C16	119.7(3)	C3'-C2'-C1'	119.5(5)	C10'-N2'-Zn1'#1	125.6(6)
C18-P1	1.830(3)	C20'-C25'	1.398(6)	C17-C16-C15	120.8(3)	C3'-C2'-C7'	114.6(5)	C11'-N2'-Zn1'#1	119.3(5)
C20-C25	1.396(4)	C20'-C21'	1.402(6)	C16-C17-C18	119.8(3)	C1'-C2'-C7'	125.7(5)	C1'-O1'-Zn1'	128.7(5)
C20-C21	1.397(5)	C20'-P1'	1.831(5)	C19-C18-C17	118.6(3)	C4'-C3'-C2'	123.4(6)	C1'-O1'-Zn1'#1	125.4(4)
C20-P1	1.829(3)	C21'-C22'	1.399(6)	C19-C18-P1	125.3(3)	C3'-C4'-C5'	117.3(5)	Zn1'-O1'-Zn1'#1	105.6(3)
C21-C22	1.400(4)	C22'-C23'	1.395(7)	C17-C18-P1	116.0(2)	C3'-C4'-C9'	122.1(7)	C13'-O2'-Zn1'	123.1(5)
C22-C23	1.395(6)	C23'-C24'	1.369(8)	C14-C19-C18	120.9(3)	C5'-C4'-C9'	120.6(7)	C20'-P1'-C18'	102.0(4)
C23-C24	1.369(7)	C24'-C25'	1.394(7)	C25-C20-C21	118.8(3)	C4'-C5'-C6'	122.3(6)	C20'-P1'-C26'	102.6(4)
C24-C25	1.392(5)	C26'-C31'	1.391(6)	C25-C20-P1	116.1(3)	C5'-C6'-C1'	120.4(5)	C18'-P1'-C26'	102.4(4)
C26-C31	1.393(5)	C26'-C27'	1.399(6)	C21-C20-P1	125.1(2)	C5'-C6'-C10'	113.8(5)	O2'-Zn1'-N1'	116.6(4)
C26-C27	1.397(4)	C26'-P1'	1.847(5)	C20-C21-C22	120.1(3)	C1'-C6'-C10'	125.7(5)	O2'-Zn1'-N2'#1	98.9(5)
C26-P1	1.846(4)	C27'-C28'	1.378(7)	C23-C22-C21	119.7(4)	N1'-C7'-C2'	127.9(6)	N1'-Zn1'-N2'#1	97.4(3)
C27-C28	1.377(5)	C28'-C29'	1.385(7)	C24-C23-C22	120.4(3)	N1'-C8'-C12'#1	109.5(8)	O2'-Zn1'-O1'	106.1(4)
C28-C29	1.384(6)	C29'-C30'	1.384(6)	C23-C24-C25	120.1(3)	N2'-C10'-C6'	127.5(6)	N1'-Zn1'-O1'	88.4(3)
C29-C30	1.385(5)	C30'-C31'	1.386(6)	C24-C25-C20	120.7(4)	N2'-C11'-C12'	109.3(6)	N2'-Zn1'-O1'#1	148.4(5)
C30-C31	1.386(5)	N1'-Zn1'	2.062(5)	C31-C26-C27	118.0(3)	C11'-C12'-C8'#1	104.0(9)	O2'-Zn1'-O1'#1	92.0(4)
N1-Zn1	2.075(3)	N2'-Zn1'#1	2.073(10)	C31-C26-P1	124.1(2)	O3'-C13'-O2'	123.8(6)	N1'-Zn1'-O1'#1	150.1(4)
N2-Zn1#1	2.108(3)	O1'-Zn1'	2.075(4)	C27-C26-P1	117.5(3)	O3'-C13'-C14'	120.1(6)	N2'#1-Zn1'-O1'#1	85.9(3)
O1-Zn1#1	2.034(2)	O1'-Zn1'#1	2.173(8)	C28-C27-C26	121.1(4)	O2'-C13'-C14'	116.0(5)	O1'-Zn1'-O1'#1	74.4(3)
O1-Zn1	2.0684(18)	O2'-Zn1'	1.971(4)	C27-C28-C29	120.4(3)	C15'-C14'-C19'	119.7(5)		
O2-Zn1	1.973(2)	Zn1'-N2'#1	2.073(10)	C28-C29-C30	119.3(4)	C15'-C14'-C13'	120.9(5)		
Zn1-O1#1	2.034(2)	Zn1'-O1'#1	2.173(8)	C29-C30-C31	120.4(4)	C19'-C14'-C13'	119.2(5)		
Zn1-N2#1	2.108(3)	O1N-C1N	1.415(5)	C30-C31-C26	120.8(3)	C14'-C15'-C16'	119.9(6)		
C1'-O1'	1.318(5)	O1M-C1M	1.393(7)	C7-N1-C8	115.7(3)	C17'-C16'-C15'	120.8(6)		

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

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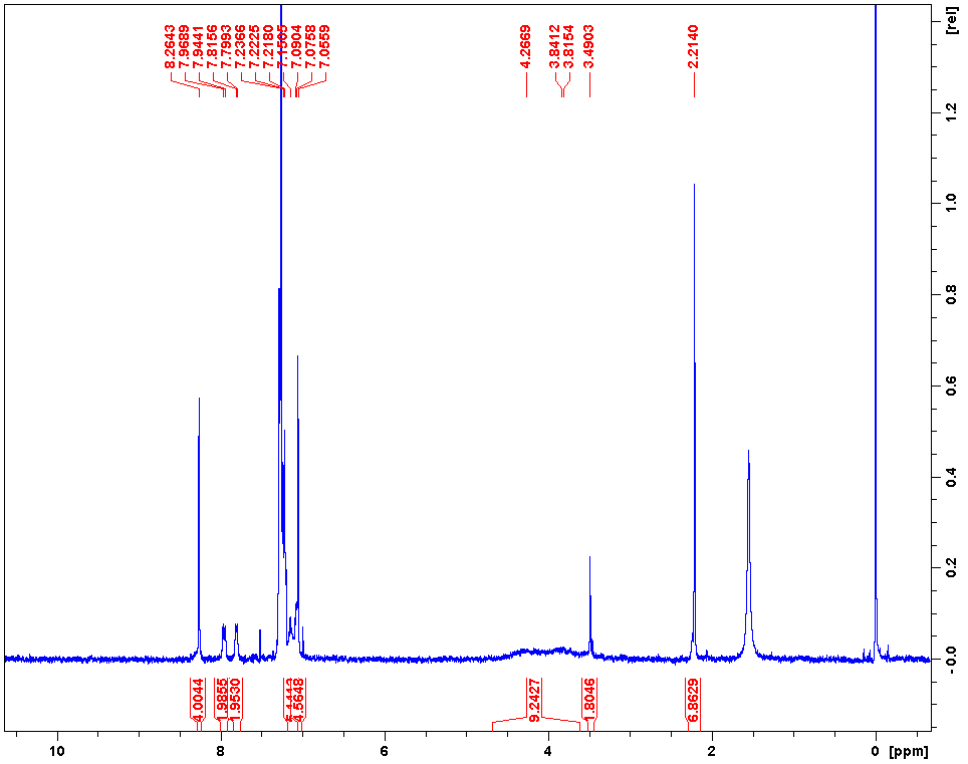
Table 3. Torsion angles [°] for SP12401_0m.

O1-C1-C2-C3	-179.2(3)	C27-C26-C31-C30	2.0(6)	C6'-C1'-C2'-C3'	4(2)	P1'-C26'-C31'-C30'	175.2(13)
C6-C1-C2-C3	1.7(5)	P1-C26-C31-C30	174.8(3)	O1'-C1'-C2'-C7'	-2(3)	C2'-C7'-N1'-C8'	-179.5(16)
O1-C1-C2-C7	1.5(6)	C2-C7-N1-C8	173.6(4)	C6'-C1'-C2'-C7'	178.4(16)	C2'-C7'-N1'-Zn1'	-1(3)
C6-C1-C2-C7	-177.6(4)	C2-C7-N1-Zn1	3.5(6)	C1'-C2'-C3'-C4'	-1(2)	C12'#1-C8'-N1'-C7'	-154.8(13)
C1-C2-C3-C4	-1.9(6)	C12#1-C8-N1-C7	129.3(4)	C7'-C2'-C3'-C4'	-176.2(15)	C12'#1-C8'-N1'-Zn1'	27.0(14)
C7-C2-C3-C4	177.4(4)	C12#1-C8-N1-Zn1	-59.9(4)	C2'-C3'-C4'-C5'	-3(2)	C6'-C10'-N2'-C11'	173.9(14)
C2-C3-C4-C5	-0.2(6)	C6-C10-N2-C11	176.4(4)	C2'-C3'-C4'-C9'	178.3(15)	C6'-C10'-N2'-Zn1'#1	11(2)
C2-C3-C4-C9	178.6(4)	C6-C10-N2-Zn1#1	5.7(6)	C3'-C4'-C5'-C6'	3(2)	C12'-C11'-N2'-C10'	-143.1(13)
C3-C4-C5-C6	2.5(6)	C12-C11-N2-C10	150.3(4)	C9'-C4'-C5'-C6'	-177.5(14)	C12'-C11'-N2'-Zn1'#1	20.8(14)
C9-C4-C5-C6	-176.3(4)	C12-C11-N2-Zn1#1	-39.3(4)	C4'-C5'-C6'-C1'	-1(2)	C6'-C1'-O1'-Zn1'	163.1(11)
C4-C5-C6-C1	-2.7(6)	C2-C1-O1-Zn1#1	148.0(3)	C4'-C5'-C6'-C10'	178.2(14)	C2'-C1'-O1'-Zn1'	-16(2)
C4-C5-C6-C10	177.0(4)	C6-C1-O1-Zn1#1	-33.0(5)	O1'-C1'-C6'-C5'	177.6(14)	C6'-C1'-O1'-Zn1'#1	-23(2)
O1-C1-C6-C5	-178.6(4)	C2-C1-O1-Zn1	-12.5(5)	C2'-C1'-C6'-C5'	-3(2)	C2'-C1'-O1'-Zn1'#1	157.7(11)
C2-C1-C6-C5	0.5(6)	C6-C1-O1-Zn1	166.6(3)	O1'-C1'-C6'-C10'	-1(2)	O3'-C13'-O2'-Zn1'	-1(2)
O1-C1-C6-C10	1.6(6)	O3-C13-O2-Zn1	-10.0(5)	C2'-C1'-C6'-C10'	178.4(15)	C14'-C13'-O2'-Zn1'	175.8(9)
C2-C1-C6-C10	-179.2(4)	C14-C13-O2-Zn1	169.7(2)	C3'-C2'-C7'-N1'	-173.4(17)	C25'-C20'-P1'-C18'	172.2(13)
C3-C2-C7-N1	-176.3(4)	C25-C20-P1-C18	171.0(3)	C1'-C2'-C7'-N1'	12(3)	C21'-C20'-P1'-C18'	10.4(13)
C1-C2-C7-N1	3.0(6)	C21-C20-P1-C18	-11.5(4)	C5'-C6'-C10'-N2'	-170.6(15)	C25'-C20'-P1'-C26'	-82.1(14)
C5-C6-C10-N2	-167.2(4)	C25-C20-P1-C26	-82.6(3)	C1'-C6'-C10'-N2'	8(3)	C21'-C20'-P1'-C26'	116.1(13)
C1-C6-C10-N2	12.6(7)	C21-C20-P1-C26	95.0(4)	N2'-C11'-C12'-C8'#1	-79.2(11)	C19'-C18'-P1'-C20'	88.2(13)
N2-C11-C12-C8#1	65.9(4)	C19-C18-P1-C20	93.1(3)	O3'-C13'-C14'-C15'	-179.8(17)	C17'-C18'-P1'-C20'	-87.0(12)
O3-C13-C14-C15	-179.1(4)	C17-C18-P1-C20	-88.5(3)	O2'-C13'-C14'-C15'	3(2)	C19'-C18'-P1'-C26'	-17.7(13)
O2-C13-C14-C15	1.1(5)	C19-C18-P1-C26	-12.4(4)	O3'-C13'-C14'-C19'	5(2)	C17'-C18'-P1'-C26'	167.1(11)
O3-C13-C14-C19	4.6(6)	C17-C18-P1-C26	166.0(3)	O2'-C13'-C14'-C19'	-171.8(14)	C31'-C26'-P1'-C20'	9.2(14)
O2-C13-C14-C19	-175.1(4)	C31-C26-P1-C20	14.8(3)	C19'-C14'-C15'-C16'	-2(3)	C27'-C26'-P1'-C20'	-168.6(12)
C19-C14-C15-C16	1.0(6)	C27-C26-P1-C20	-172.3(3)	C13'-C14'-C15'-C16'	-177.6(17)	C31'-C26'-P1'-C18'	114.7(13)
C13-C14-C15-C16	-175.2(4)	C31-C26-P1-C18	120.9(3)	C14'-C15'-C16'-C17'	6(3)	C27'-C26'-P1'-C18'	-63.1(14)
C14-C15-C16-C17	-1.6(6)	C27-C26-P1-C18	-66.3(3)	C15'-C16'-C17'-C18'	-8(3)	C13'-O2'-Zn1'-N1'	-18.2(13)
C15-C16-C17-C18	1.9(6)	C13-O2-Zn1-O1#1	156.5(3)	C16'-C17'-C18'-C19'	6(2)	C13'-O2'-Zn1'-N2'#1	-121.2(11)
C16-C17-C18-C19	-1.6(6)	C13-O2-Zn1-O1	77.3(3)	C16'-C17'-C18'-P1'	-178.7(15)	C13'-O2'-Zn1'-O1'	78.3(12)
C16-C17-C18-P1	179.8(3)	C13-O2-Zn1-N1	-17.7(3)	C17'-C18'-C19'-C14'	-2(2)	C13'-O2'-Zn1'-O1'#1	152.6(11)
C15-C14-C19-C18	-0.7(6)	C13-O2-Zn1-N2#1	-114.4(3)	P1'-C18'-C19'-C14'	-177.5(11)	C7'-N1'-Zn1'-O2'	97.0(13)
C13-C14-C19-C18	175.6(4)	C1-O1-Zn1-O2	-100.9(3)	C15'-C14'-C19'-C18'	1(2)	C8'-N1'-Zn1'-O2'	-84.9(11)
C17-C18-C19-C14	1.0(6)	Zn1#1-O1-Zn1-O2	95.45(14)	C13'-C14'-C19'-C18'	176.0(13)	C7'-N1'-Zn1'-N2'#1	-159.2(13)
P1-C18-C19-C14	179.4(3)	C1-O1-Zn1-O1#1	163.7(4)	C25'-C20'-C21'-C22'	16(2)	C8'-N1'-Zn1'-N2'#1	19.0(11)
C25-C20-C21-C22	-5.6(7)	Zn1#1-O1-Zn1-O1#1	0.0	P1'-C20'-C21'-C22'	178.0(15)	C7'-N1'-Zn1'-O1'	-10.3(14)
P1-C20-C21-C22	176.9(4)	C1-O1-Zn1-N1	14.0(3)	C20'-C21'-C22'-C23'	-9(3)	C8'-N1'-Zn1'-O1'	167.8(11)
C20-C21-C22-C23	5.3(8)	Zn1#1-O1-Zn1-N1	-149.64(14)	C21'-C22'-C23'-C24'	-6(3)	C7'-N1'-Zn1'-O1'#1	-64.4(16)
C21-C22-C23-C24	-1.2(8)	C1-O1-Zn1-N2#1	104.9(4)	C22'-C23'-C24'-C25'	13(4)	C8'-N1'-Zn1'-O1'#1	113.7(10)
C22-C23-C24-C25	-2.4(8)	Zn1#1-O1-Zn1-N2#1	-58.7(3)	C23'-C24'-C25'-C20'	-6(4)	C1'-O1'-Zn1'-O2'	-97.6(12)
C23-C24-C25-C20	2.0(8)	C7-N1-Zn1-O2	98.0(3)	C21'-C20'-C25'-C24'	-9(3)	Zn1'#1-O1'-Zn1'-O2'	87.5(5)
C21-C20-C25-C24	2.0(7)	C8-N1-Zn1-O2	-71.8(3)	P1'-C20'-C25'-C24'	-171.8(18)	C1'-O1'-Zn1'-N1'	19.7(13)
P1-C20-C25-C24	179.7(4)	C7-N1-Zn1-O1#1	-71.7(4)	C31'-C26'-C27'-C28'	3(3)	Zn1'#1-O1'-Zn1'-N1'	-155.2(6)
C31-C26-C27-C28	-2.7(6)	C8-N1-Zn1-O1#1	118.5(3)	P1'-C26'-C27'-C28'	-179.0(15)	C1'-O1'-Zn1'-N2'#1	121.4(12)
P1-C26-C27-C28	-175.9(4)	C7-N1-Zn1-O1	-9.1(3)	C26'-C27'-C28'-C29'	4(3)	Zn1'#1-O1'-Zn1'-N2'#1	-53.5(8)
C26-C27-C28-C29	1.3(8)	C8-N1-Zn1-O1	-178.9(3)	C27'-C28'-C29'-C30'	-8(3)	C1'-O1'-Zn1'-O1'#1	174.9(16)
C27-C28-C29-C30	0.8(8)	C7-N1-Zn1-N2#1	-161.7(3)	C28'-C29'-C30'-C31'	4(3)	Zn1'#1-O1'-Zn1'-O1'#1	0.0
C28-C29-C30-C31	-1.5(8)	C8-N1-Zn1-N2#1	28.5(3)	C29'-C30'-C31'-C26'	4(3)		
C29-C30-C31-C26	0.1(7)	O1'-C1'-C2'-C3'	-176.8(14)	C27'-C26'-C31'-C30'	-7(2)		

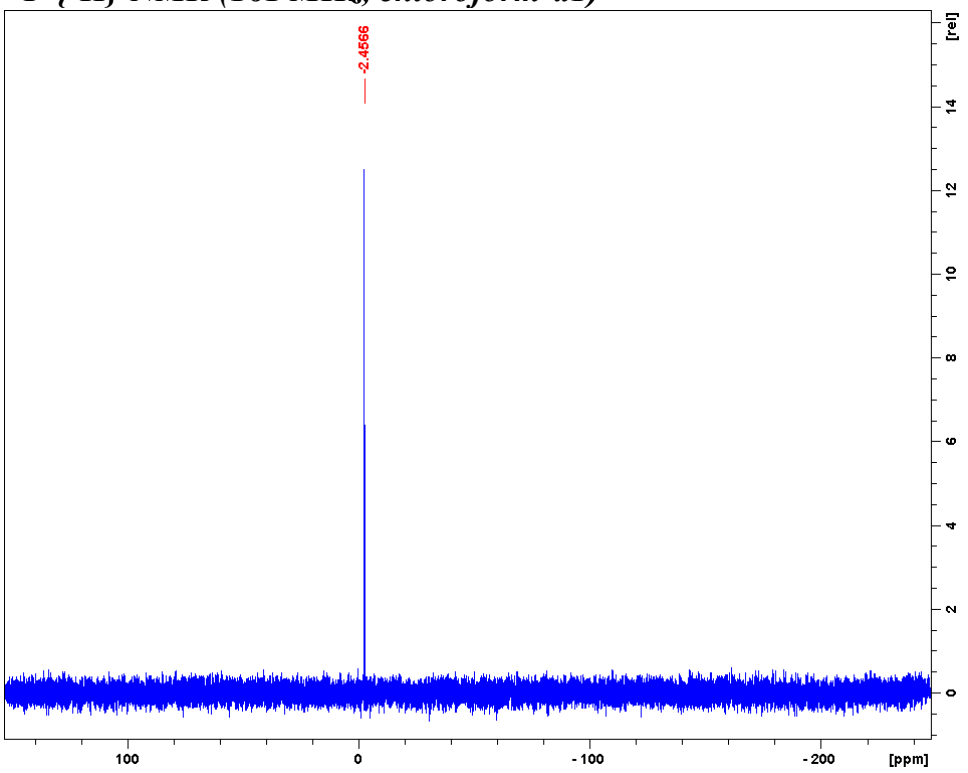
Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y+1, -z+2

8E’

^{1}H-NMR (400 MHz, chloroform-d$_1$)



^{31}P-{^{1}H}-NMR (161 MHz, chloroform-d1)



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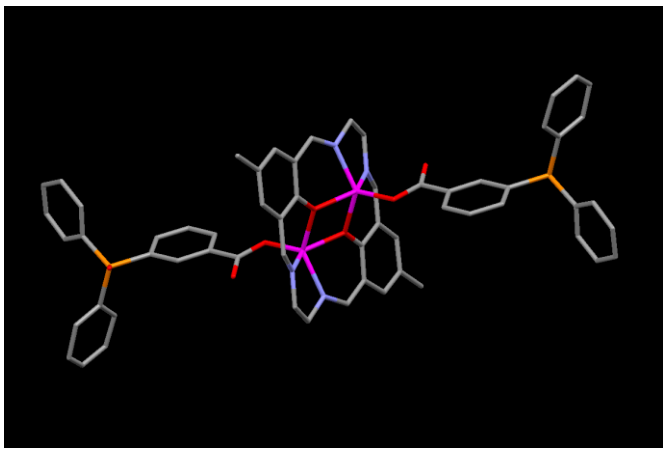
Single Crystal X-Ray Diffraction Data **8E´ dioxide**



Representation of **8E'** dioxide

Table 1. Crystal data and structure refinement for SP132_0m.

Identification code	SP132_0m	
Empirical formula	C60 H50 N4 O8 P2 Zn2	
Formula weight	1147.72	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 18.819(5) Å	α = 90.00 °
	b = 6.9218(16) Å	β = 100.119(13) °
	c = 19.998(5) Å	γ = 90.00 °
Volume	2564.5(11) Å^3	
Z	2	
Density (calculated)	1.486 Mg/m^3	
Absorption coefficient	1.061 mm^{-1}	
F(000)	1184	
Crystal size	0.08 x 0.06 x 0.02 mm^3	
Theta range for data collection	3.12 to 31.32 °.	
Index ranges	$-27 \le h \le 11$, $-10 \le k \le 9$, $-24 \le l \le 28$	
Reflections collected	7959	
Independent reflections	3735 [R_{int} = 0.0743]	
Completeness to theta =31.32 °	0.948 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9791 and 0.9200	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7959 / 2273 / 711	
Goodness-of-fit on F_2	0.975	
Final R indices [I>2sigma(I)]	R_1 = 0.0608 , wR_2 = 0.1452	
R indices (all data)	R_1 = 0.1543 , wR_2 = 0.1865	
Largest diff. peak and hole	0.747 and -0.557 e·Å^{-3}	

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- SP132_0m

The phosphine group is disordered over three positions which were initially refined free with combined occupancies leading to 100%. Afterwards they were modeled with a 45:35:20 and restrained to have equal distances and angles within the three groups. Displacement parameters of all atoms in the disordered the phosphine groups were restrained. Moreover, the distance between Zn1 and the three equivalent carboxylate oxygen atoms of the disordered phosphine group was restrained to be equal. As a result of the disordered phosphines, C10 is disordered over two positions (C10 and C10') which was refined free leading to an occupancy of 31.6 (2)% and constrained to have the same displacement parameters. Distances between neighboring equivalent atoms restrained to be equal.

Table 2. Bond lengths [Å] and angles [°] for SP132_0m.

Bond lengths----				Angles----------					
C1-O1	1.301(4)	P1Y-C17Y	1.796(3)	O1-C1-C6	120.9(3)	O4-P1-C25	116.1(4)	C26Y-C27Y-C28Y	119.91(13)
C1-C6	1.406(5)	C19Y-C20Y	1.3909(9)	O1-C1-C2	119.3(3)	O4-P1-C19	112.5(5)	C27Y-C28Y-C29Y	119.82(15)
C1-C2	1.411(5)	C19Y-C24Y	1.3912(10)	C6-C1-C2	119.8(3)	C25-P1-C19	105.2(3)	C30Y-C29Y-C28Y	119.77(16)
C2-C3	1.408(5)	C20Y-C21Y	1.3902(10)	C3-C2-C1	118.4(3)	O4-P1-C17	111.0(3)	C25Y-C30Y-C29Y	119.83(14)
C2-C8	1.448(5)	C21Y-C22Y	1.3903(10)	C3-C2-C8	118.3(3)	C25-P1-C17	104.0(2)	O3Y-C12Y-O2Y	124.71(16)
C3-C4	1.366(6)	C22Y-C23Y	1.3904(10)	C1-C2-C8	123.1(3)	C19-P1-C17	107.3(2)	O3Y-C12Y-C13Y	118.77(15)
C4-C5	1.377(5)	C23Y-C24Y	1.3902(10)	C4-C3-C2	121.8(3)	C20-C19-C24	120.0	O2Y-C12Y-C13Y	116.43(15)
C4-C7	1.534(6)	C25Y-C26Y	1.3899(9)	C3-C4-C5	118.9(3)	C20-C19-P1	122.2(3)	C14Y-C13Y-C18Y	119.34(11)
C5-C6	1.390(5)	C25Y-C30Y	1.3904(9)	C3-C4-C7	120.8(4)	C24-C19-P1	117.8(3)	C14Y-C13Y-C12Y	121.88(13)
C6-C11	1.461(5)	C26Y-C27Y	1.3901(9)	C5-C4-C7	120.3(4)	C19-C20-C21	120.0	C18Y-C13Y-C12Y	118.76(13)
C8-N1	1.264(4)	C27Y-C28Y	1.3903(9)	C4-C5-C6	122.3(4)	C22-C21-C20	120.0	C15Y-C14Y-C13Y	120.98(13)
C9-N1	1.458(5)	C28Y-C29Y	1.3906(10)	C5-C6-C1	118.6(3)	C21-C22-C23	120.0	C14Y-C15Y-C16Y	119.76(13)
C9-C10	1.493(7)	C29Y-C30Y	1.3904(9)	C5-C6-C11	119.3(3)	C24-C23-C22	120.0	C15Y-C16Y-C17Y	120.71(12)
C9-C10'	1.498(6)	C12Y-O3Y	1.2313(9)	C1-C6-C11	122.0(3)	C23-C24-C19	120.0	C18Y-C17Y-C16Y	117.78(12)
C10-N2	1.489(6)	C12Y-O2Y	1.2580(9)	N1-C8-C2	124.5(3)	C26-C25-C30	120.0	C18Y-C17Y-P1Y	118.0(2)
C10'-N2	1.488(5)	C12Y-C13Y	1.5120(9)	N1-C9-C10	114.4(5)	C26-C25-P1	124.7(2)	C16Y-C17Y-P1Y	123.9(2)
C11-N2#1	1.275(4)	C13Y-C14Y	1.3799(9)	N1-C9-C10'	113.3(3)	C30-C25-P1	115.2(2)	C13Y-C18Y-C17Y	121.24(12)
N1-Zn1	2.033(3)	C13Y-C18Y	1.3886(9)	C10-C9-C10'	23.2(7)	C27-C26-C25	120.0	C12Y-O2Y-Zn1	121.0(5)
N2-C11#1	1.275(4)	C14Y-C15Y	1.3728(9)	N2-C10-C9	111.5(4)	C26-C27-C28	120.0	O4X-P1X-C25X	116.0(4)
N2-Zn1	2.035(3)	C15Y-C16Y	1.3899(9)	N2-C10'-C9	111.3(4)	C29-C28-C27	120.0	O4X-P1X-C19X	112.5(5)
O1-Zn1	2.015(3)	C16Y-C17Y	1.4059(9)	N2-C11-C6#1	125.7(3)	C30-C29-C28	120.0	C25X-P1X-C19X	105.3(3)
O1-Zn1#1	2.017(2)	C17Y-C18Y	1.3969(9)	C8-N1-C9	121.7(3)	C29-C30-C25	120.0	O4X-P1X-C17X	110.9(4)
Zn1-O2	1.967(3)	P1X-O4X	1.426(7)	C8-N1-Zn1	126.2(2)	O3-C12-O2	124.8	C25X-P1X-C17X	104.0(2)
Zn1-O2X	1.969(4)	P1X-C25X	1.772(4)	C9-N1-Zn1	112.1(2)	O3-C12-C13	118.8	C19X-P1X-C17X	107.4(3)
Zn1-O2Y	1.969(4)	P1X-C19X	1.791(5)	C11-N2-C10'#1	124.9(4)	O2-C12-C13	116.4	C20X-C19X-C24X	119.92(14)
Zn1-O1#1	2.017(2)	P1X-C17X	1.796(3)	C11-N2-C10#1	116.2(4)	C14-C13-C18	119.4	C20X-C19X-P1X	122.2(3)
P1-O4	1.425(7)	C19X-C20X	1.3902(9)	C10'-N2-C10	23.3(7)	C14-C13-C12	121.9	C24X-C19X-P1X	117.8(3)
P1-C25	1.772(4)	C19X-C24X	1.3904(9)	C11-N2-Zn1#1	127.3(3)	C18-C13-C12	118.7	C19X-C20X-C21X	119.92(13)
P1-C19	1.792(5)	C20X-C21X	1.3903(10)	C10'-N2-Zn1	107.6(3)	C15-C14-C13	121.0	C22X-C21X-C20X	119.93(14)
P1-C17	1.796(3)	C21X-C22X	1.3902(10)	C10-N2-Zn1	114.2(3)	C14-C15-C16	119.8	C23X-C22X-C21X	119.88(16)
C19-C20	1.3900	C22X-C23X	1.3902(9)	C1-O1-Zn1	125.8(2)	C15-C16-C17	120.7	C22X-C23X-C24X	119.92(14)
C19-C24	1.3900	C23X-C24X	1.3902(10)	C1-O1-Zn1#1	128.3(2)	C18-C17-C16	117.9	C23X-C24X-C19X	119.93(13)
C20-C21	1.3900	C25X-C26X	1.3903(9)	Zn1-O1-Zn1#1	105.88(11)	C18-C17-P1	118.12(16)	C26X-C25X-C30X	119.93(11)
C21-C22	1.3900	C25X-C30X	1.3904(9)	O2-Zn1-O2X	5.2(9)	C16-C17-P1	123.98(17)	C26X-C25X-P1X	124.6(2)
C22-C23	1.3900	C26X-C27X	1.3902(10)	O2-Zn1-O2Y	2.3(10)	C13-C18-C17	121.2	C30X-C25X-P1X	115.1(2)
C23-C24	1.3900	C27X-C28X	1.3905(10)	O2X-Zn1-O2Y	7.3(17)	C12-O2-Zn1	117.8(3)	C27X-C26X-C25X	120.00(13)
C25-C26	1.3900	C28X-C29X	1.3906(10)	O2-Zn1-O1	111.1(3)	O4Y-P1Y-C25Y	116.0(4)	C26X-C27X-C28X	119.82(15)
C25-C30	1.3900	C29X-C30X	1.3901(10)	O2X-Zn1-O1	112.9(14)	O4Y-P1Y-C19Y	112.4(5)	C27X-C28X-C29X	119.74(17)
C26-C27	1.3900	C12X-O3X	1.2313(10)	O2Y-Zn1-O1	109.2(8)	C25Y-P1Y-C19Y	105.3(3)	C30X-C29X-C28X	119.80(16)
C27-C28	1.3900	C12X-O2X	1.2580(9)	O2-Zn1-O1#1	109.0(2)	O4Y-P1Y-C17Y	111.0(3)	C29X-C30X-C25X	119.96(14)
C28-C29	1.3900	C12X-C13X	1.5120(9)	O2X-Zn1-O1#1	104.6(4)	C25Y-P1Y-C17Y	104.1(2)	O3X-C12X-O2X	124.72(18)
C29-C30	1.3900	C13X-C14X	1.3801(9)	O2Y-Zn1-O1#1	110.1(4)	C19Y-P1Y-C17Y	107.3(3)	O3X-C12X-C13X	118.77(16)
C12-O3	1.2310	C13X-C18X	1.3889(9)	O1-Zn1-O1#1	74.12(11)	C20Y-C19Y-C24Y	119.66(14)	O2X-C12X-C13X	116.43(15)
C12-O2	1.2578	C14X-C15X	1.3729(10)	O2-Zn1-N1	117.5(2)	C20Y-C19Y-P1Y	121.9(3)	C14X-C13X-C18X	119.25(12)
C12-C13	1.5119	C15X-C16X	1.3900(9)	O2X-Zn1-N1	122.2(4)	C24Y-C19Y-P1Y	117.5(3)	C14X-C13X-C12X	121.86(16)
C13-C14	1.3798	C16X-C17X	1.4063(9)	O2Y-Zn1-N1	116.2(5)	C21Y-C20Y-C19Y	119.94(14)	C18X-C13X-C12X	118.71(14)
C13-C18	1.3885	C17X-C18X	1.3974(9)	O1-Zn1-N1	84.49(11)	C20Y-C21Y-C22Y	119.93(15)	C15X-C14X-C13X	120.93(15)
C14-C15	1.3728			O1-Zn1-N1#1	133.17(11)	C21Y-C22Y-C23Y	119.78(15)	C14X-C15X-C16X	119.72(15)
C15-C16	1.3899			O2-Zn1-N2	112.2(3)	C24Y-C23Y-C22Y	119.88(15)	C15X-C16X-C17X	120.64(13)
C16-C17	1.4056			O2X-Zn1-N2	109.6(14)	C23Y-C24Y-C19Y	119.93(14)	C18X-C17X-C16X	117.62(11)
C17-C18	1.3965			O2Y-Zn1-N2	114.2(8)	C26Y-C25Y-C30Y	119.95(11)	C18X-C17X-P1X	117.9(2)
P1Y-O4Y	1.425(7)			O1-Zn1-N2	136.02(12)	C26Y-C25Y-P1Y	124.8(2)	C16X-C17X-P1X	123.8(2)
P1Y-C25Y	1.772(4)			O1-Zn1-N2#1	84.83(11)	C30Y-C25Y-P1Y	115.2(2)	C13X-C18X-C17X	121.11(15)
P1Y-C19Y	1.792(5)			N1-Zn1-N2	82.59(11)	C25Y-C26Y-C27Y	120.03(12)	C12X-O2X-Zn1	110.5(6)

Symmetry transformations used to generate equivalent atoms: #1 -x, -y+0, -z

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Table 3. Torsion angles [°] for SP132_0m.

O1-C1-C2-C3	179.6(3)	C1-O1-Zn1-N2	-117.5(3)	C19-P1-C25-C30	172.4(3)	C20Y-C19Y-C24Y-C23Y	-8.2(19)	C24X-C19X-C20X-C21X	-4(4)
C6-C1-C2-C3	0.4(5)	Zn1#1-O1-Zn1-N2	64.55(18)	C17-P1-C25-C30	-74.9(3)	P1Y-C19Y-C24Y-C23Y	-177.3(12)	P1X-C19X-C20X-C21X	179(2)
O1-C1-C2-C8	3.5(5)	C8-N1-Zn1-O2	-84.9(5)	C30-C25-C26-C27	0.0	O4Y-P1Y-C25Y-C26Y	-161.5(10)	C19X-C20X-C21X-C22X	-2(4)
C6-C1-C2-C8	-175.8(3)	C9-N1-Zn1-O2	93.5(4)	P1-C25-C26-C27	-176.04(16)	C19Y-P1Y-C25Y-C26Y	-36.5(10)	C20X-C21X-C22X-C23X	7(3)
C1-C2-C3-C4	3.0(5)	C8-N1-Zn1-O2X	-87.6(17)	C25-C26-C27-C28	0.0	C17Y-P1Y-C25Y-C26Y	76.3(10)	C21X-C22X-C23X-C24X	-6(4)
C8-C2-C3-C4	179.3(4)	C9-N1-Zn1-O2X	90.8(17)	C26-C27-C28-C29	0.0	O4Y-P1Y-C25Y-C30Y	22.3(13)	C22X-C23X-C24X-C19X	-1(4)
C2-C3-C4-C5	-3.0(6)	C8-N1-Zn1-O2Y	-82.7(10)	C27-C28-C29-C30	0.0	C19Y-P1Y-C25Y-C30Y	147.3(12)	C20X-C19X-C24X-C23X	6(3)
C2-C3-C4-C7	178.1(4)	C9-N1-Zn1-O2Y	95.7(9)	C28-C29-C30-C25	0.0	C17Y-P1Y-C25Y-C30Y	-99.9(12)	P1X-C19X-C24X-C23X	-178(2)
C3-C4-C5-C6	-0.3(6)	C8-N1-Zn1-O1	26.0(3)	C26-C25-C30-C29	0.0	C30Y-C25Y-C26Y-C27Y	-1(2)	O4X-P1X-C25X-C26X	-114.8(14)
C7-C4-C5-C6	178.6(4)	C9-N1-Zn1-O1	-155.5(2)	P1-C25-C30-C29	176.40(15)	P1Y-C25Y-C26Y-C27Y	-176.6(11)	C19X-P1X-C25X-C26X	10.3(13)
C4-C5-C6-C1	3.5(6)	C8-N1-Zn1-O1#1	88.1(3)	O3-C12-C13-C14	-167.3	C25Y-C26Y-C27Y-C28Y	1(2)	C17X-P1X-C25X-C26X	123.1(13)
C4-C5-C6-C11	-178.2(4)	C9-N1-Zn1-O1#1	-93.4(3)	O2-C12-C13-C14	13.3	C26Y-C27Y-C28Y-C29Y	-6(2)	O4X-P1X-C25X-C30X	57.9(14)
O1-C1-C6-C5	177.2(3)	C8-N1-Zn1-N2	163.9(3)	O3-C12-C13-C18	12.0	C27Y-C28Y-C29Y-C30Y	10(2)	C19X-P1X-C25X-C30X	-177.0(13)
C2-C1-C6-C5	-3.5(5)	C9-N1-Zn1-N2	-17.7(2)	O2-C12-C13-C18	-167.3	C26Y-C25Y-C30Y-C29Y	5(2)	C17X-P1X-C25X-C30X	-64.2(13)
O1-C1-C6-C11	-1.0(5)	C11#1-N2-Zn1-O2	88.1(4)	C18-C13-C14-C15	1.7	P1Y-C25Y-C30Y-C29Y	-179.1(12)	C30X-C25X-C26X-C27X	-2(2)
C2-C1-C6-C11	178.3(3)	C10'-N2-Zn1-O2	-86.0(5)	C12-C13-C14-C15	-178.9	C28Y-C29Y-C30Y-C25Y	-9(2)	P1X-C25X-C26X-C27X	170.1(18)
C3-C2-C8-N1	162.5(3)	C10-N2-Zn1-O2	-110.0(11)	C13-C14-C15-C16	-0.9	O3Y-C12Y-C13Y-C14Y	-155(2)	C25X-C26X-C27X-C28X	-3(3)
C1-C2-C8-N1	-21.4(5)	C11#1-N2-Zn1-O2X	83.3(6)	C14-C15-C16-C17	0.7	O2Y-C12Y-C13Y-C14Y	28(2)	C26X-C27X-C28X-C29X	9(3)
N1-C9-C10-N2	-20.1(19)	C10'-N2-Zn1-O2X	-90.8(6)	C15-C16-C17-C18	-1.3	O3Y-C12Y-C13Y-C18Y	23(2)	C27X-C28X-C29X-C30X	-10(3)
C10'-C9-C10-N2	72.5(7)	C10-N2-Zn1-O2X	-114.8(11)	C15-C16-C17-P1	-178.8(2)	O2Y-C12Y-C13Y-C18Y	-153.5(19)	C28X-C29X-C30X-C25X	5(3)
N1-C9-C10'-N2	25.6(9)	C11#1-N2-Zn1-O2Y	89.4(6)	O4-P1-C17-C18	22.3(5)	C18Y-C13Y-C14Y-C15Y	2(3)	C26X-C25X-C30X-C29X	1(3)
C10-C9-C10'-N2	-72.3(7)	C10'-N2-Zn1-O2Y	-84.7(6)	C25-P1-C17-C18	147.84(19)	C12Y-C13Y-C14Y-C15Y	-179.2(18)	P1X-C25X-C30X-C29X	-172(2)
C5-C6-C11-N2#1	166.9(4)	C10-N2-Zn1-O2Y	-108.7(12)	C19-P1-C17-C18	-101.0(3)	C13Y-C14Y-C15Y-C16Y	-4(3)	O3X-C12X-C13X-C14X	173(3)
C1-C6-C11-N2#1	-14.9(6)	C11#1-N2-Zn1-O1	-81.0(4)	O4-P1-C17-C16	-160.1(5)	C14Y-C15Y-C16Y-C17Y	1(3)	O2X-C12X-C13X-C14X	-11(3)
C2-C8-N1-C9	179.6(3)	C10'-N2-Zn1-O1	104.9(4)	C25-P1-C17-C16	-34.6(4)	C15Y-C16Y-C17Y-C18Y	3(2)	O3X-C12X-C13X-C18X	-3(3)
C2-C8-N1-Zn1	-2.1(5)	C10-N2-Zn1-O1	80.9(11)	C19-P1-C17-C16	76.6(3)	C15Y-C16Y-C17Y-P1Y	176.2(16)	O2X-C12X-C13X-C18X	174(3)
C10-C9-N1-C8	-155.7(10)	C11#1-N2-Zn1-O1#1	-20.3(4)	C14-C13-C18-C17	-2.3	O4Y-P1Y-C17Y-C18Y	18.9(12)	C18X-C13X-C14X-C15X	-2(3)
C10'-C9-N1-C8	178.9(5)	C10'-N2-Zn1-O1#1	165.6(4)	C12-C13-C18-C17	178.3	C25Y-P1Y-C17Y-C18Y	144.3(11)	C12X-C13X-C14X-C15X	-177(3)
C10-C9-N1-Zn1	25.8(11)	C10-N2-Zn1-O1#1	141.6(11)	C16-C17-C18-C13	2.1	C19Y-P1Y-C17Y-C18Y	-104.3(11)	C13X-C14X-C15X-C16X	6(4)
C10'-C9-N1-Zn1	0.4(6)	C11#1-N2-Zn1-N1	-155.1(4)	P1-C17-C18-C13	179.8(2)	O4Y-P1Y-C17Y-C16Y	-154.7(14)	C14X-C15X-C16X-C17X	-2(4)
C9-C10'-N2-C11#1	147.0(5)	C10'-N2-Zn1-N1	30.8(4)	O3-C12-O2-Zn1	0.9(4)	C25Y-P1Y-C17Y-C16Y	-29.3(14)	C15X-C16X-C17X-C18X	-5(2)
C9-C10'-N2-C10	72.0(7)	C10-N2-Zn1-N1	6.8(11)	C13-C12-O2-Zn1	-179.9(4)	C19Y-P1Y-C17Y-C16Y	82.0(14)	C15X-C16X-C17X-P1X	166(2)
C9-C10'-N2-Zn1	-38.7(8)	O4-P1-C19-C20	-153.7(5)	O2X-Zn1-O2-C12	136(15)	C14Y-C13Y-C18Y-C17Y	2(3)	O4X-P1X-C17X-C18X	33.7(13)
C9-C10-N2-C11#1	169.2(10)	C25-P1-C19-C20	79.1(5)	O2Y-Zn1-O2-C12	-74(13)	C12Y-C13Y-C18Y-C17Y	-176.7(13)	C25X-P1X-C17X-C18X	159.1(12)

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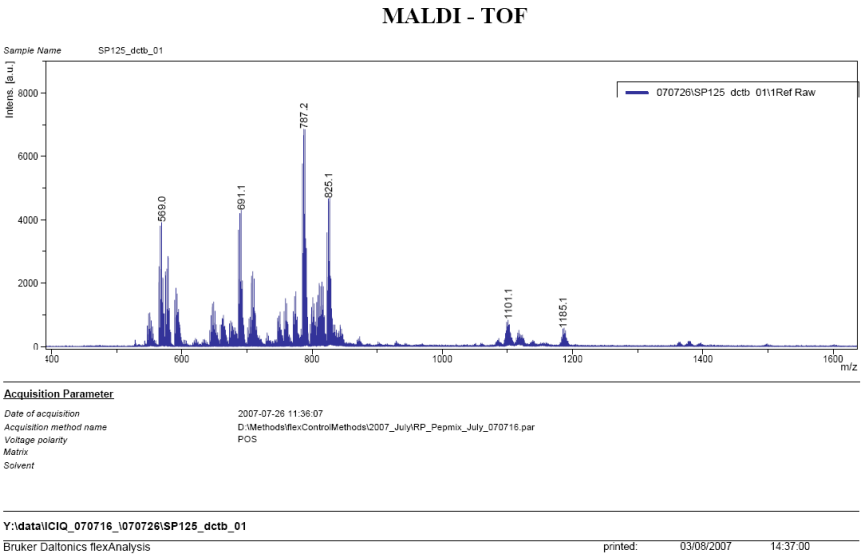
C9-C10-N2-C10'	-72.9(7)	C17-P1-C19-C20	-31.3(5)	O1-Zn1-O2-C12	-112.3(3)	C16Y-C17Y-C18Y-C13Y	-4(2)	C19X-P1X-C17X-C18X	-89.6(12)
C9-C10-N2-Zn1	5.1(19)	O4-P1-C19-C24	28.0(5)	O1#1-Zn1-O2-C12	168.0(2)	P1Y-C17Y-C18Y-C13Y	-178.2(13)	O4X-P1X-C17X-C16X	-137.2(15)
C6-C1-O1-Zn1	-144.5(3)	C25-P1-C19-C24	-99.3(4)	N1-Zn1-O2-C12	-17.4(5)	O3Y-C12Y-O2Y-Zn1	7(3)	C25X-P1X-C17X-C16X	-11.8(14)
C2-C1-O1-Zn1	36.2(4)	C17-P1-C19-C24	150.4(4)	N2-Zn1-O2-C12	75.8(4)	C13Y-C12Y-O2Y-Zn1	-176.3(14)	C19X-P1X-C17X-C16X	99.5(15)
C6-C1-O1-Zn1#1	33.0(4)	C24-C19-C20-C21	0.0	O4Y-P1Y-C19Y-C20Y	-118.8(10)	O2-Zn1-O2Y-C12Y	93(13)	C14X-C13X-C18X-C17X	-6(3)
C2-C1-O1-Zn1#1	-146.3(3)	P1-C19-C20-C21	-178.3(5)	C25Y-P1Y-C19Y-C20Y	114.0(10)	O2X-Zn1-O2Y-C12Y	114(14)	C12X-C13X-C18X-C17X	170(2)
C1-O1-Zn1-O2	73.3(3)	C19-C20-C21-C22	0.0	C17Y-P1Y-C19Y-C20Y	3.5(10)	O1-Zn1-O2Y-C12Y	-125.0(18)	C16X-C17X-C18X-C13X	9.3(16)
Zn1#1-O1-Zn1-O2	-104.7(2)	C20-C21-C22-C23	0.0	O4Y-P1Y-C19Y-C24Y	50.1(10)	O1#1-Zn1-O2Y-C12Y	155.4(17)	P1X-C17X-C18X-C13X	-162.1(16)
C1-O1-Zn1-O2X	78.5(6)	C21-C22-C23-C24	0.0	C25Y-P1Y-C19Y-C24Y	-77.1(9)	N1-Zn1-O2Y-C12Y	-32(2)	O3X-C12X-O2X-Zn1	-4(4)
Zn1#1-O1-Zn1-O2X	-99.4(6)	C22-C23-C24-C19	0.0	C17Y-P1Y-C19Y-C24Y	172.4(9)	N2-Zn1-O2Y-C12Y	62(2)	C13X-C12X-O2X-Zn1	180(2)
C1-O1-Zn1-O2Y	71.8(6)	C20-C19-C24-C23	0.0	C24Y-C19Y-C20Y-C21Y	8(2)	O4X-P1X-C19X-C20X	-153.8(18)	O2-Zn1-O2X-C12X	-31(13)
Zn1#1-O1-Zn1-O2Y	-106.2(5)	P1-C19-C24-C23	178.4(5)	P1Y-C19Y-C20Y-C21Y	176.4(12)	C25X-P1X-C19X-C20X	78.9(18)	O2Y-Zn1-O2X-C12X	-40(10)
C1-O1-Zn1-O1#1	178.0(3)	O4-P1-C25-C26	-136.4(4)	C19Y-C20Y-C21Y-C22Y	-7(2)	C17X-P1X-C19X-C20X	-31.5(18)	O1-Zn1-O2X-C12X	-101(3)
Zn1#1-O1-Zn1-O1#1	0.0	C19-P1-C25-C26	-11.4(3)	C20Y-C21Y-C22Y-C23Y	7(2)	O4X-P1X-C19X-C24X	29.9(18)	O1#1-Zn1-O2X-C12X	-180(2)
C1-O1-Zn1-N1	-44.1(3)	C17-P1-C25-C26	101.4(2)	C21Y-C22Y-C23Y-C24Y	-8(2)	C25X-P1X-C19X-C24X	-97.3(17)	N1-Zn1-O2X-C12X	-3(4)
Zn1#1-O1-Zn1-N1	137.91(13)	O4-P1-C25-C30	47.4(5)	C22Y-C23Y-C24Y-C19Y	8(2)	C17X-P1X-C19X-C24X	152.2(17)	N2-Zn1-O2X-C12X	90(3)

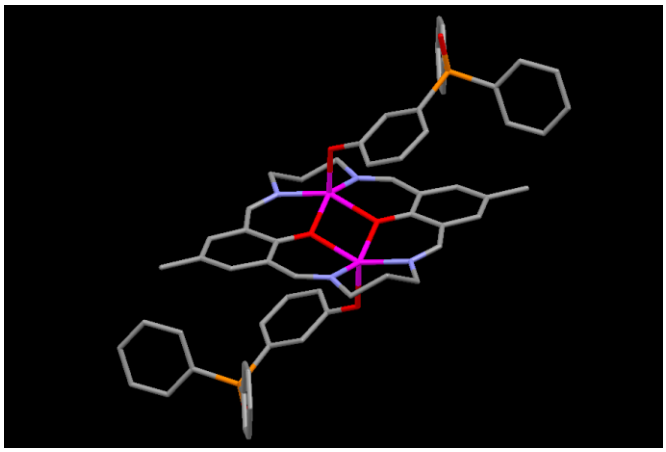
Symmetry transformations used to generate equivalent atoms: #1 -x, -y+0, -z

9D’

MALDI-TOF-MS



Single Crystal X-Ray Diffraction Data 9D´ dioxide



Representation of **9D’** dioxide

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Table 1. Crystal data and structure refinement for sp125p21c.

Identification code	sp125p21c	
Empirical formula	C60 H54 N4 O6 P2 Zn2	
Formula weight	1119.75	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 8.4567(3) Å	α= 90.00 °
	b = 34.8441(9) Å	β = 97.9190(10) °
	c = 8.4433(2) Å	γ = 90.00 °
Volume	2464.23(12) Å^3	
Z	2	
Density (calculated)	1.509 Mg/m^3	
Absorption coefficient	1.099 mm^{-1}	
F(000)	1160	
Crystal size	0.08 x 0.08 x 0.03 mm^3	
Theta range for data collection	3.00 to 40.02 °.	
Index ranges	$-15 \le h \le 9$, $-61 \le k \le 6$, $-14 \le l \le 14$	
Reflections collected	14185	
Independent reflections	12913 [R_{int}= 0.0321]	
Completeness to theta =40.02 °	0.928 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9678 and 0.9172	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14185 / 0 / 335	
Goodness-of-fit on F_2	1.115	
Final R indices [I>2sigma(I)]	R_1 = 0.0371 , wR_2 = 0.0947	
R indices (all data)	R_1 = 0.0413 , wR_2 = 0.0967	
Largest diff. peak and hole	1.266 and -0.400 e·Å^{-3}	

Table 2. Bond lengths [Å] and angles [°] for sp125p21c.

Bond lengths----		Angles----------			
C1-N1	1.4722(13)	N1-C1-C2	112.36(9)	C10-N1-Zn1#1	124.85(7)
C1-C2	1.5185(17)	C1-C2-C3	113.17(10)	C1-N1-Zn1	120.24(7)
C2-C3	1.5189(16)	N2-C3-C2	112.98(8)	C4-N2-C3	114.58(8)
C3-N2	1.4745(13)	N2-C4-C5	128.25(9)	C4-N2-Zn1	123.87(7)
C4-N2	1.2840(12)	C6-C5-C12	120.68(9)	C3-N2-Zn1	121.20(6)
C4-C5	1.4515(14)	C6-C5-C4	114.47(8)	C12-O1-Zn1	127.67(6)
C5-C6	1.4036(13)	C12-C5-C4	124.85(8)	C12-O1-Zn1#1	127.80(6)
C5-C12	1.4227(13)	C7-C6-C5	122.91(9)	Zn1-O1-Zn1#1	104.41(3)
C6-C7	1.3873(14)	C6-C7-C8	116.49(8)	C13-O2-Zn1	117.65(6)
C7-C8	1.3925(14)	C6-C7-C11	121.93(9)	O3-P1-C15	114.45(5)
C7-C11	1.5078(14)	C8-C7-C11	121.58(9)	O3-P1-C25	110.49(5)
C8-C9	1.4025(13)	C7-C8-C9	122.83(9)	C15-P1-C25	106.39(4)
C9-C12	1.4238(13)	C8-C9-C12	120.64(8)	O3-P1-C19	111.18(4)
C9-C10	1.4498(13)	C8-C9-C10	114.73(8)	C15-P1-C19	106.75(5)
C10-N1#1	1.2859(13)	C12-C9-C10	124.63(8)	C25-P1-C19	107.20(5)
C12-O1	1.3075(11)	N1-C10-C9#1	127.68(9)	O2-Zn1-O1	102.81(3)
C13-O2	1.3208(12)	O1-C12-C5	122.02(8)	O2-Zn1-N2	107.14(3)
C13-C14	1.4076(13)	O1-C12-C9	121.59(8)	O1-Zn1-N2	88.69(3)
C13-C18	1.4101(14)	C5-C12-C9	116.39(8)	O2-Zn1-O1#1	103.31(3)
C14-C15	1.3956(13)	O2-C13-C14	120.83(8)	O1-Zn1-O1#1	75.60(3)
C15-C16	1.3992(14)	O2-C13-C18	121.75(8)	N2-Zn1-O1#1	148.16(3)
C15-P1	1.7984(9)	C14-C13-C18	117.42(9)	O2-Zn1-N1	105.18(3)
C16-C17	1.3924(14)	C15-C14-C13	121.42(8)	O1-Zn1-N1	149.70(3)
C17-C18	1.3864(15)	C14-C15-C16	120.16(8)	N2-Zn1-N1	93.94(3)
C19-C20	1.3941(14)	C14-C15-P1	120.13(7)	O1-Zn1-N1#1	86.84(3)
C19-C24	1.3990(15)	C16-C15-P1	119.37(7)		
C19-P1	1.8074(10)	C17-C16-C15	118.83(9)		
C20-C21	1.3944(17)	C18-C17-C16	121.20(9)		
C21-C22	1.387(2)	C17-C18-C13	120.94(9)		
C22-C23	1.3917(18)	C20-C19-C24	119.66(10)		
C23-C24	1.3905(16)	C20-C19-P1	117.82(8)		
C25-C30	1.3963(14)	C24-C19-P1	122.52(7)		
C25-C26	1.3971(15)	C19-C20-C21	119.85(11)		
C25-P1	1.8066(10)	C22-C21-C20	120.03(11)		
C26-C27	1.3962(16)	C21-C22-C23	120.61(11)		
C27-C28	1.3859(19)	C24-C23-C22	119.40(11)		
C28-C29	1.3907(19)	C23-C24-C19	120.45(10)		
C29-C30	1.3909(15)	C30-C25-C26	119.47(9)		
N1-C10#1	1.2859(13)	C30-C25-P1	117.16(8)		
N1-Zn1	2.0875(9)	C26-C25-P1	123.36(8)		
N2-Zn1	2.0705(8)	C27-C26-C25	119.89(11)		
O1-Zn1	2.0703(7)	C28-C27-C26	120.30(11)		
O1-Zn1#1	2.0855(7)	C27-C28-C29	119.96(11)		
O2-Zn1	1.9481(8)	C28-C29-C30	120.07(11)		
O3-P1	1.5267(8)	C29-C30-C25	120.27(10)		
Zn1-O1#1	2.0855(7)	C10-N1-C1#1	114.37(8)		

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

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Table 3. Torsion angles [°] for sp125p21c.

N1-C1-C2-C3	-73.63(12)	C21-C22-C23-C24	-0.39(18)	C20-C19-P1-O3	-13.44(10)
C1-C2-C3-N2	71.84(12)	C22-C23-C24-C19	-0.22(17)	C24-C19-P1-O3	167.28(8)
N2-C4-C5-C6	-172.93(11)	C20-C19-C24-C23	0.86(16)	C20-C19-P1-C15	-138.91(8)
N2-C4-C5-C12	7.35(17)	P1-C19-C24-C23	-179.87(8)	C24-C19-P1-C15	41.81(9)
C12-C5-C6-C7	-1.80(16)	C30-C25-C26-C27	-1.50(18)	C20-C19-P1-C25	107.41(9)
C4-C5-C6-C7	178.47(10)	P1-C25-C26-C27	177.67(10)	C24-C19-P1-C25	-71.87(9)
C5-C6-C7-C8	0.41(16)	C25-C26-C27-C28	0.8(2)	C13-O2-Zn1-O1	-85.23(7)
C5-C6-C7-C11	179.89(10)	C26-C27-C28-C29	0.9(2)	C13-O2-Zn1-N2	-177.84(7)
C6-C7-C8-C9	1.87(15)	C27-C28-C29-C30	-1.9(2)	C13-O2-Zn1-O1#1	-7.26(7)
C11-C7-C8-C9	-177.62(10)	C28-C29-C30-C25	1.25(19)	C13-O2-Zn1-N1	83.06(7)
C7-C8-C9-C12	-2.75(15)	C26-C25-C30-C29	0.47(17)	C12-O1-Zn1-O2	-83.24(8)
C7-C8-C9-C10	177.35(10)	P1-C25-C30-C29	-178.75(9)	Zn1#1-O1-Zn1-O2	100.68(4)
C8-C9-C10-N1#1	-171.51(10)	C2-C1-N1-C10#1	-139.41(10)	C12-O1-Zn1-N2	24.05(8)
C12-C9-C10-N1#1	8.60(17)	C2-C1-N1-Zn1	48.64(13)	Zn1#1-O1-Zn1-N2	-152.04(4)
C6-C5-C12-O1	-179.54(9)	C5-C4-N2-C3	178.88(10)	C12-O1-Zn1-O1#1	176.09(10)
C4-C5-C12-O1	0.16(15)	C5-C4-N2-Zn1	5.51(16)	Zn1#1-O1-Zn1-O1#1	0.0
C6-C5-C12-C9	0.91(14)	C2-C3-N2-C4	140.74(10)	C12-O1-Zn1-N1	119.61(9)
C4-C5-C12-C9	-179.39(9)	C2-C3-N2-Zn1	-45.70(12)	Zn1#1-O1-Zn1-N1	-56.47(7)
C8-C9-C12-O1	-178.30(9)	C5-C12-O1-Zn1	-19.72(13)	C4-N2-Zn1-O2	86.83(9)
C10-C9-C12-O1	1.59(15)	C9-C12-O1-Zn1	159.82(7)	C3-N2-Zn1-O2	-86.12(8)
C8-C9-C12-C5	1.26(14)	C5-C12-O1-Zn1#1	155.48(7)	C4-N2-Zn1-O1	-16.18(9)
C10-C9-C12-C5	-178.85(9)	C9-C12-O1-Zn1#1	-24.98(13)	C3-N2-Zn1-O1	170.87(8)
O2-C13-C14-C15	178.07(9)	C14-C13-O2-Zn1	-106.39(9)	C4-N2-Zn1-O1#1	-75.61(11)
C18-C13-C14-C15	-2.32(14)	C18-C13-O2-Zn1	74.02(11)	C3-N2-Zn1-O1#1	111.44(9)
C13-C14-C15-C16	1.25(15)	C14-C15-P1-O3	-91.87(9)	C4-N2-Zn1-N1	-165.96(9)
C13-C14-C15-P1	174.53(7)	C16-C15-P1-O3	81.46(9)	C3-N2-Zn1-N1	21.09(9)
C14-C15-C16-C17	0.63(16)	C14-C15-P1-C25	145.83(8)	C10#1-N1-Zn1-O2	-84.65(9)
P1-C15-C16-C17	-172.69(8)	C16-C15-P1-C25	-40.85(10)	C1-N1-Zn1-O2	86.40(9)
C15-C16-C17-C18	-1.39(17)	C14-C15-P1-C19	31.59(9)	C10#1-N1-Zn1-O1	72.25(12)
C16-C17-C18-C13	0.27(17)	C16-C15-P1-C19	-155.08(8)	C1-N1-Zn1-O1	-116.69(9)
O2-C13-C18-C17	-178.84(10)	C30-C25-P1-O3	18.80(10)	C10#1-N1-Zn1-N2	166.40(9)
C14-C13-C18-C17	1.56(15)	C26-C25-P1-O3	-160.38(9)	C1-N1-Zn1-N2	-22.55(9)
C24-C19-C20-C21	-0.88(17)	C30-C25-P1-C15	143.58(9)	C10#1-N1-Zn1-O1#1	18.29(9)
P1-C19-C20-C21	179.82(10)	C26-C25-P1-C15	-35.61(11)	C1-N1-Zn1-O1#1	-170.66(9)
C19-C20-C21-C22	0.28(19)	C30-C25-P1-C19	-102.49(9)		
C20-C21-C22-C23	0.4(2)	C26-C25-P1-C19	78.32(10)		

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

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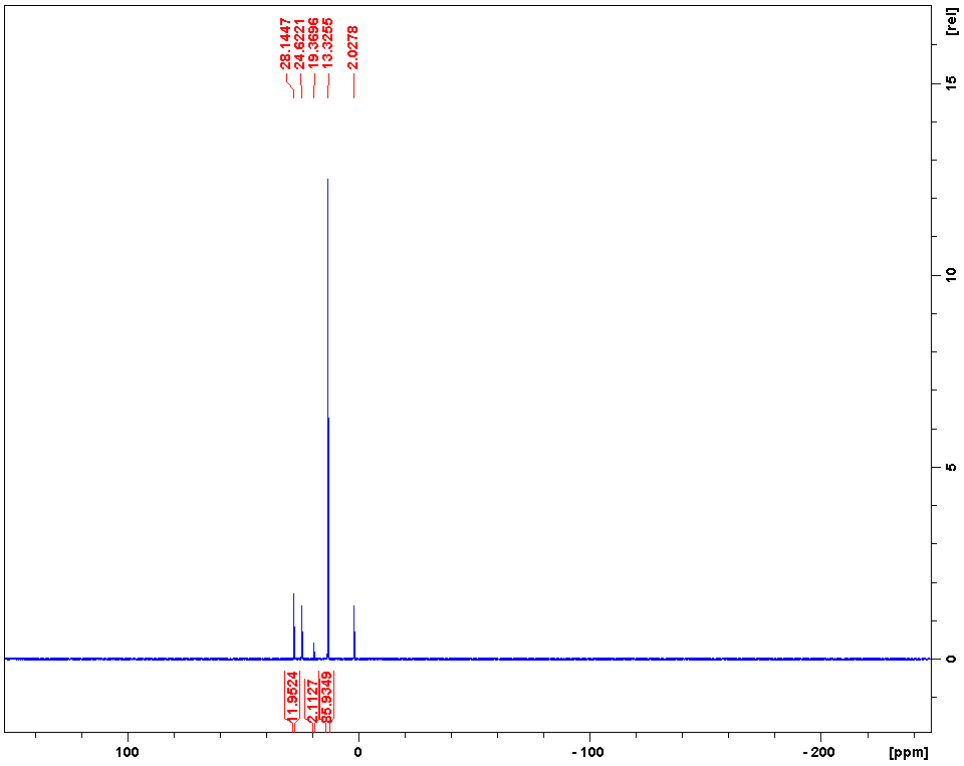
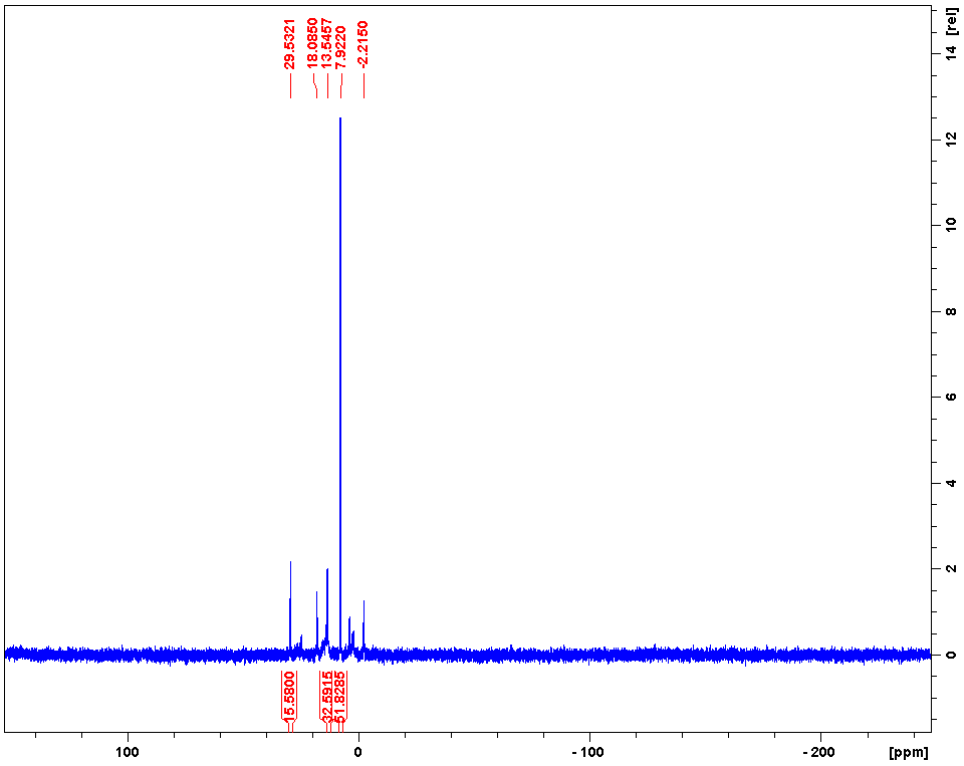
Metal templated assembled diphosphines

10A and 11A

10A ^{31}P-{^{1}H}-NMR (161 MHz, CD_2Cl_2)



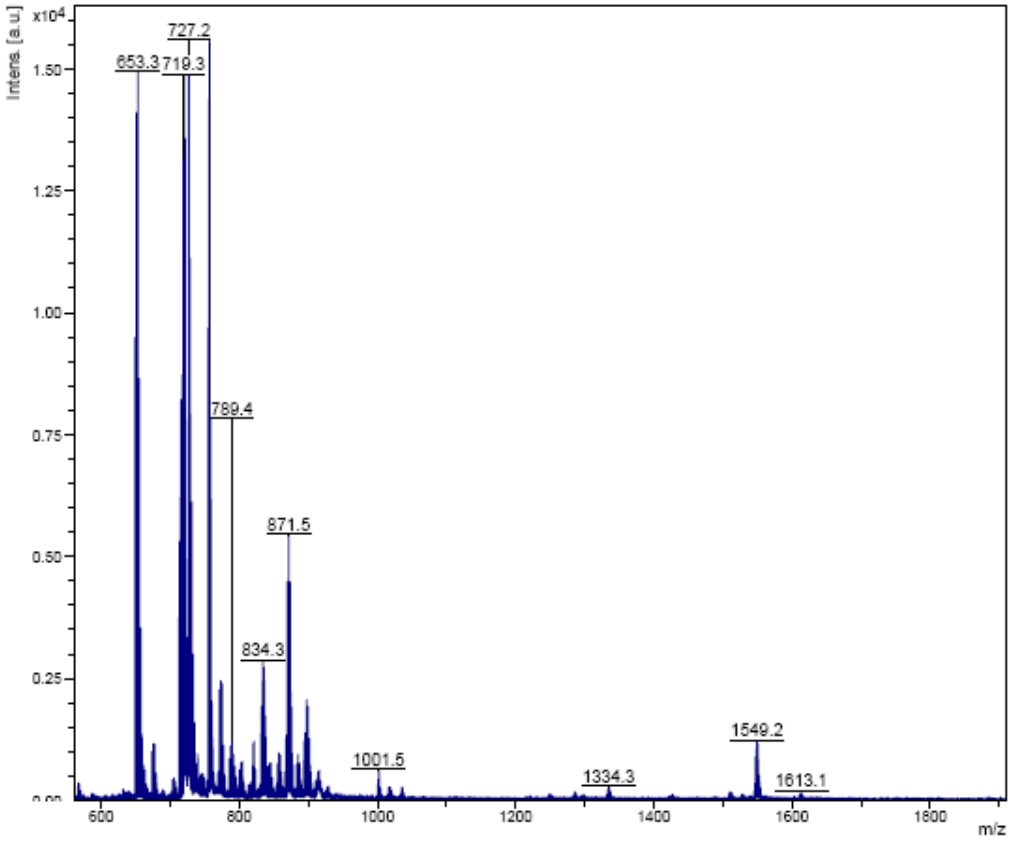
11A ^{31}P-{^{1}H}-NMR (161 MHz, CD_2Cl_2)



MALDI-TOF-MS

Y:\data\ICIQ_080107\080128\SP169\0_D14\1

Comment 1 DCTB/CH2Cl2
Comment 2 MALDI+



Acquisition Parameter

Date of acquisition	2008-01-28 16:36:00
Acquisition method name	D:\Methods\flexControlMethods\december07\RP_Pepmix_070831-noemi.par
Spectrum type	TOF
Parent ion mass for ms/ms spectra	1000
Parent mass + PCIS upper mass limit	0
Parent mass - PCIS lower mass limit	0
CID valve/mode	false

Instrument Info

User	tof-user
Instrument	FLEX-PC
Instrument type	autoflex

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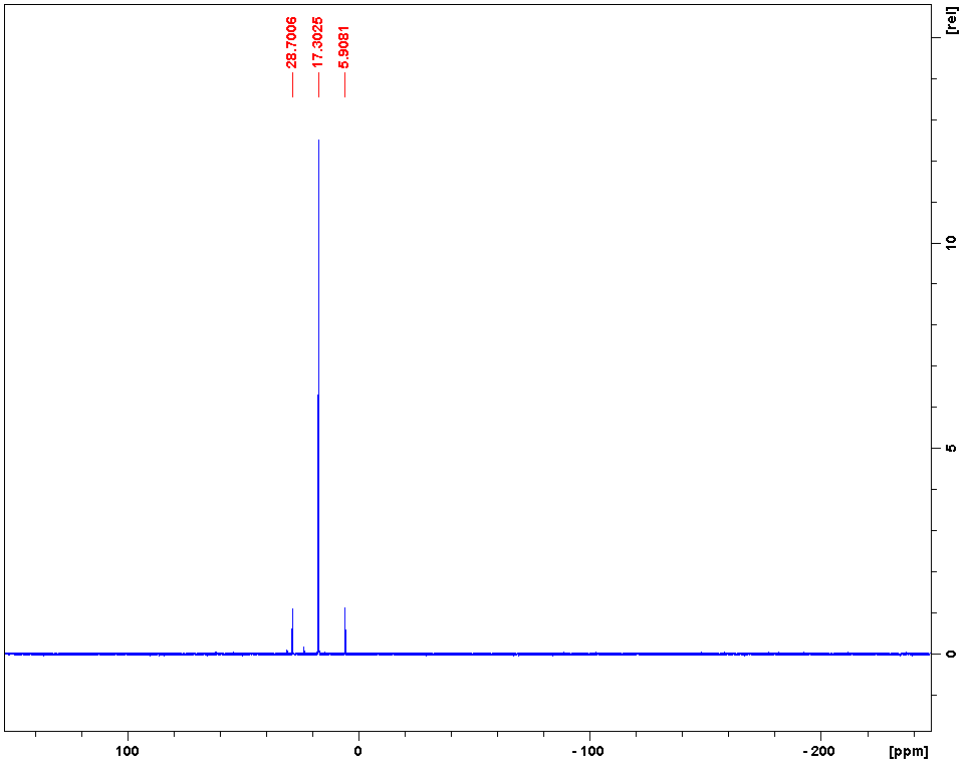
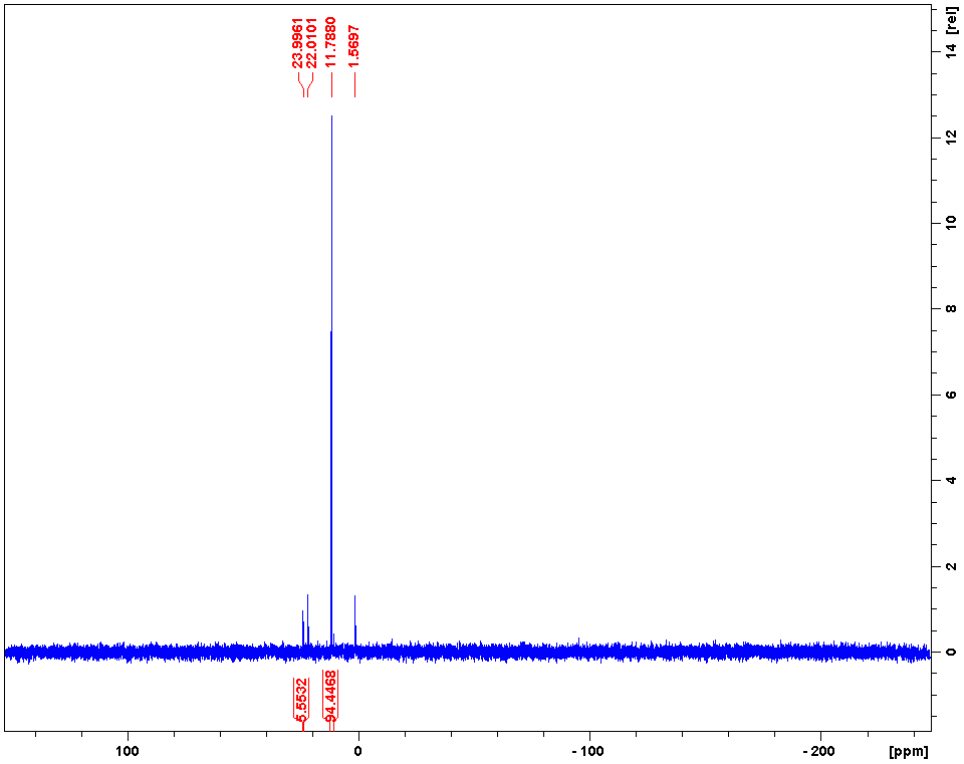
10B and 11B

10B ^{31}P-{^{1}H}-NMR (161 MHz, CD_2Cl_2)



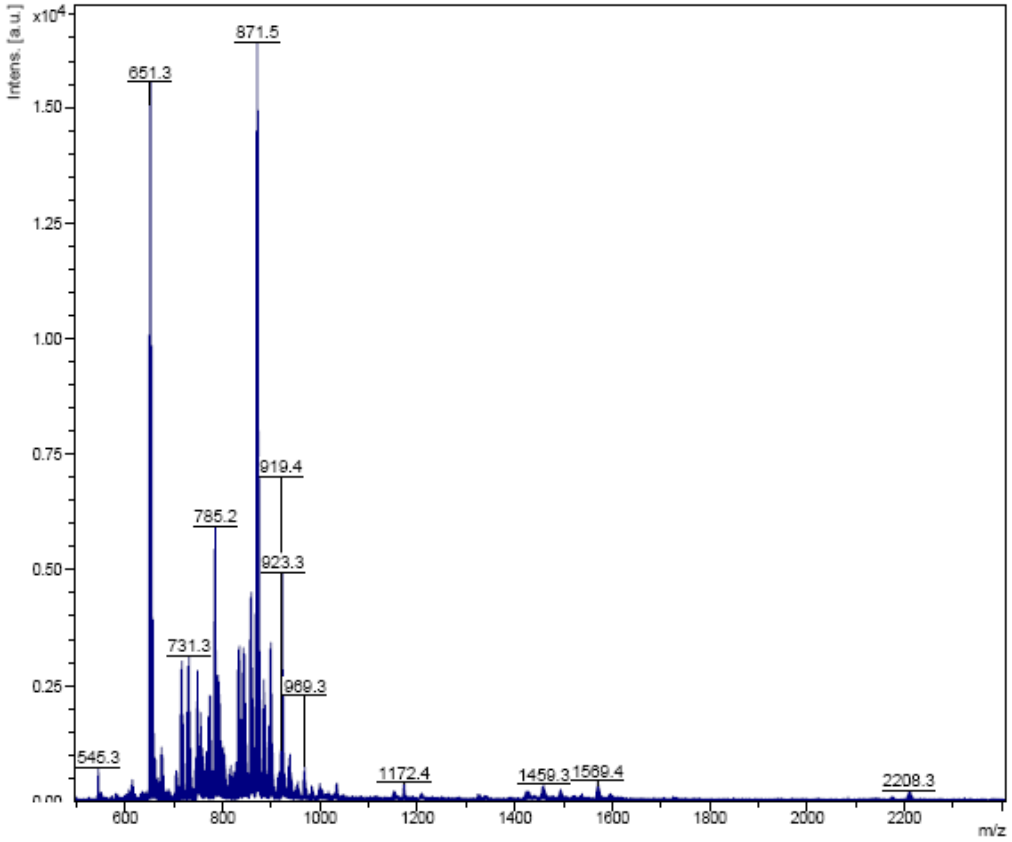
11B ^{31}P-{^{1}H}-NMR (161 MHz, CD_2Cl_2)



MALDI-TOF-MS

Y:\data\ICIQ_080107\080128\SP171\0_D10\1

Comment 1 DCTB/CH2Cl2
Comment 2 MALDI+



Acquisition Parameter

Date of acquisition	2008-01-28 18:37:57
Acquisition method name	D:\Methods\flexControlMethods\december07\RP_Pepmix_070831-noemi.par
Spectrum type	TOF
Parent ion mass for ms/ms spectra	1000
Parent mass + PCIS upper mass limit	0
Parent mass - PCIS lower mass limit	0
CID valve/mode	false

Instrument Info

User	tof-user
Instrument	FLEX-PC
Instrument type	autoflex

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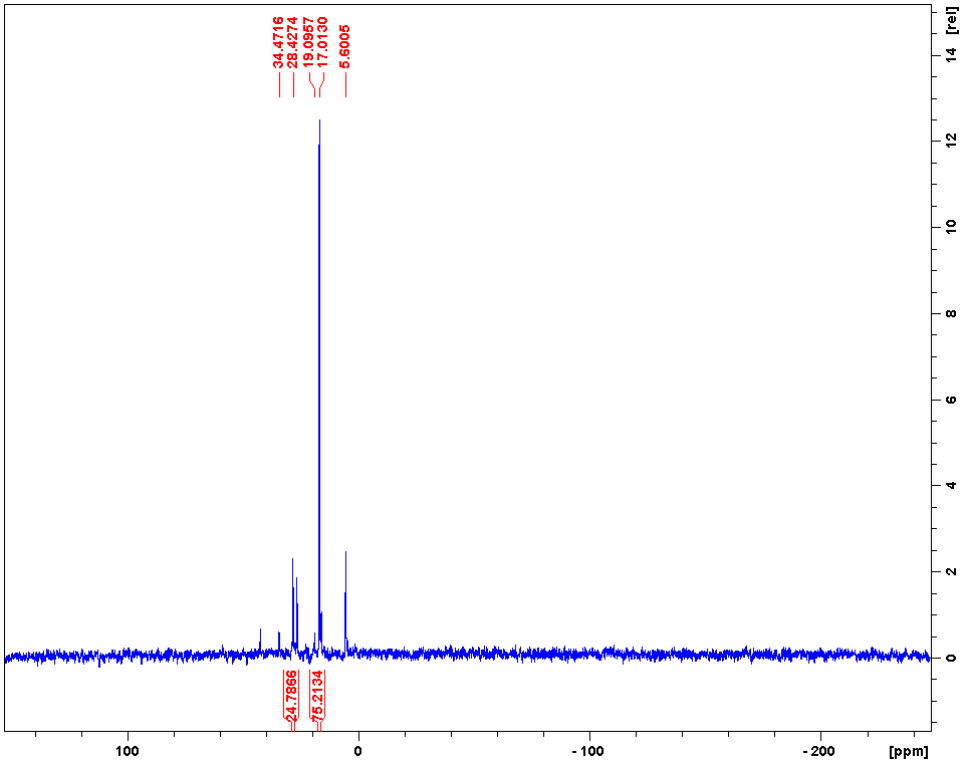
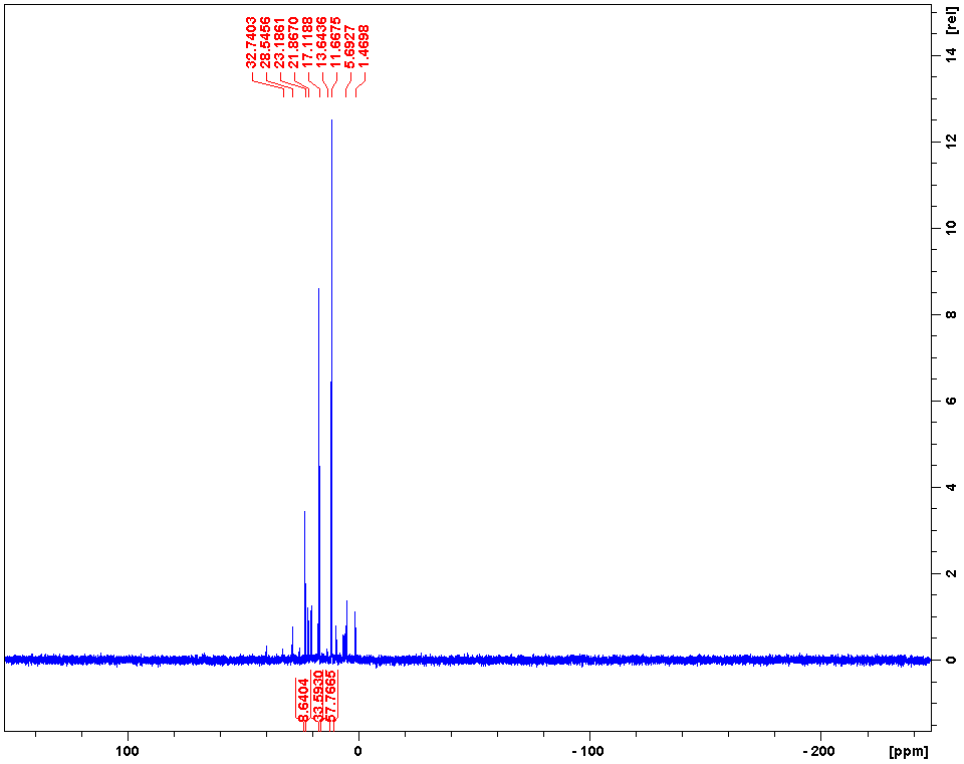
10D and 11D

10D ^{31}P-{^{1}H}-NMR (161 MHz, CD_2Cl_2)



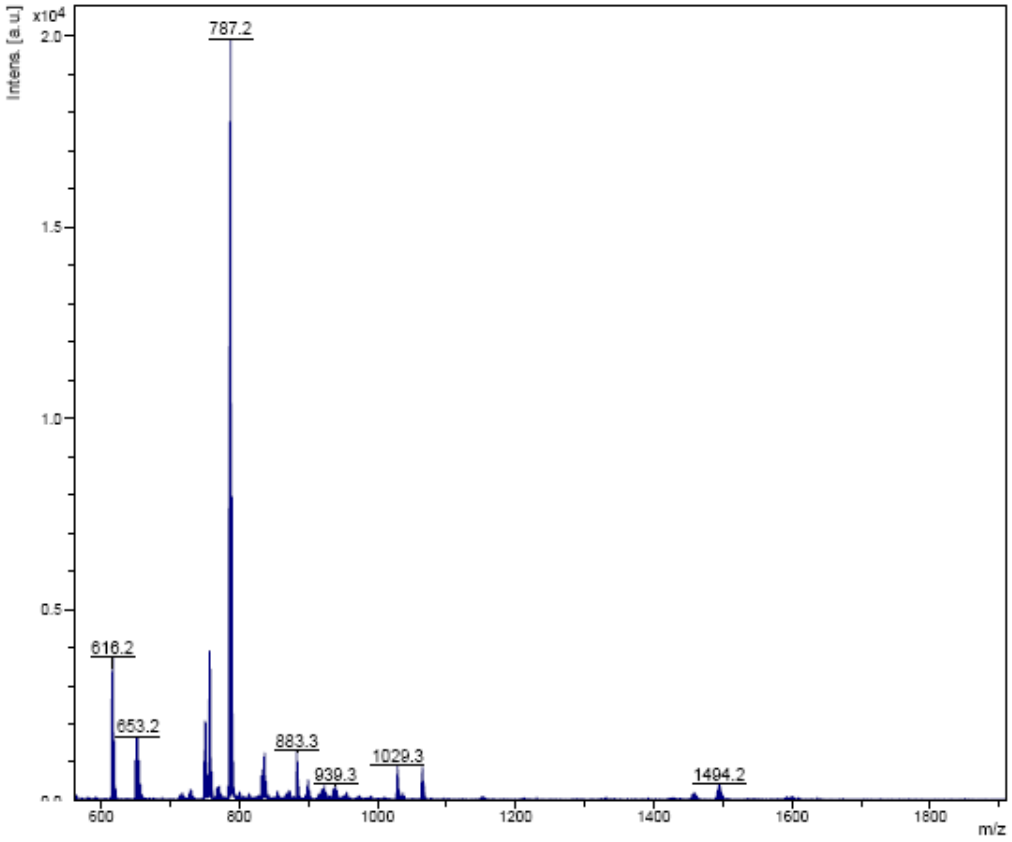
11D ^{31}P-{^{1}H}-NMR (161 MHz, CD_2Cl_2)



MALDI-TOF-MS

Y:\data\ICIQ_080107\080128\SP170\0_D12\1

Comment 1 DCTB/CH2Cl2
Comment 2 MALDI+



Acquisition Parameter

Date of acquisition	2008-01-28 16:36:51
Acquisition method name	D:\Methods\flexControlMethods\december07\RP_Pepmix_070831-noemi.par
Spectrum type	TOF
Parent ion mass for ms/ms spectra	1000
Parent mass + PCIS upper mass limit	0
Parent mass - PCIS lower mass limit	0
CID valve/mode	false

Instrument Info

User	tof-user
Instrument	FLEX-PC
Instrument type	autoflex

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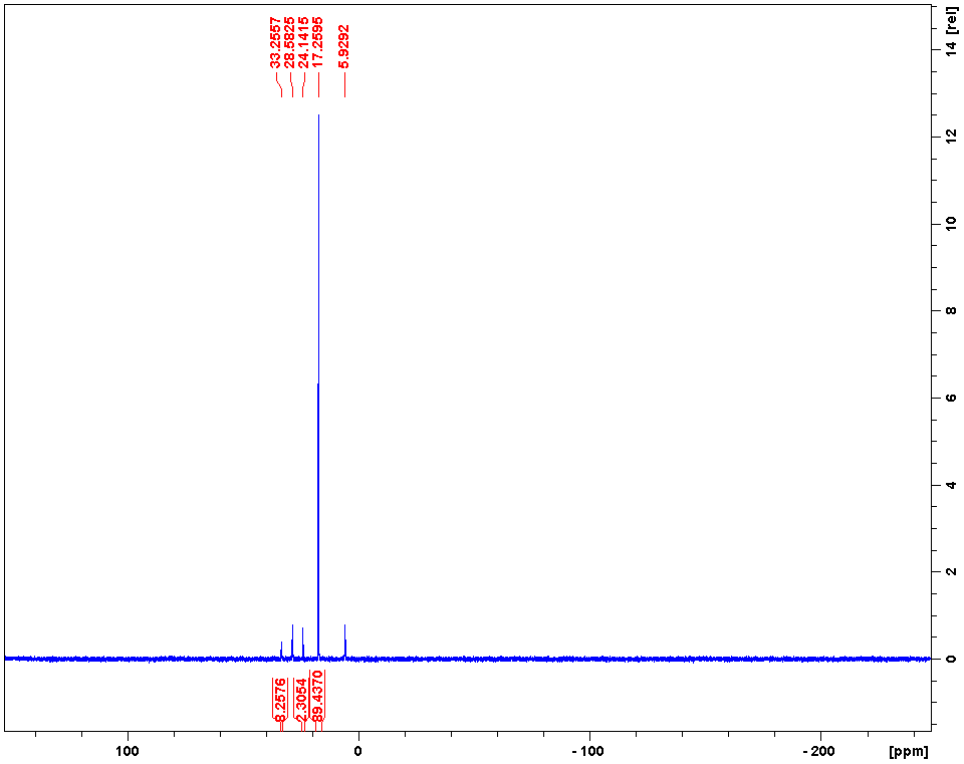
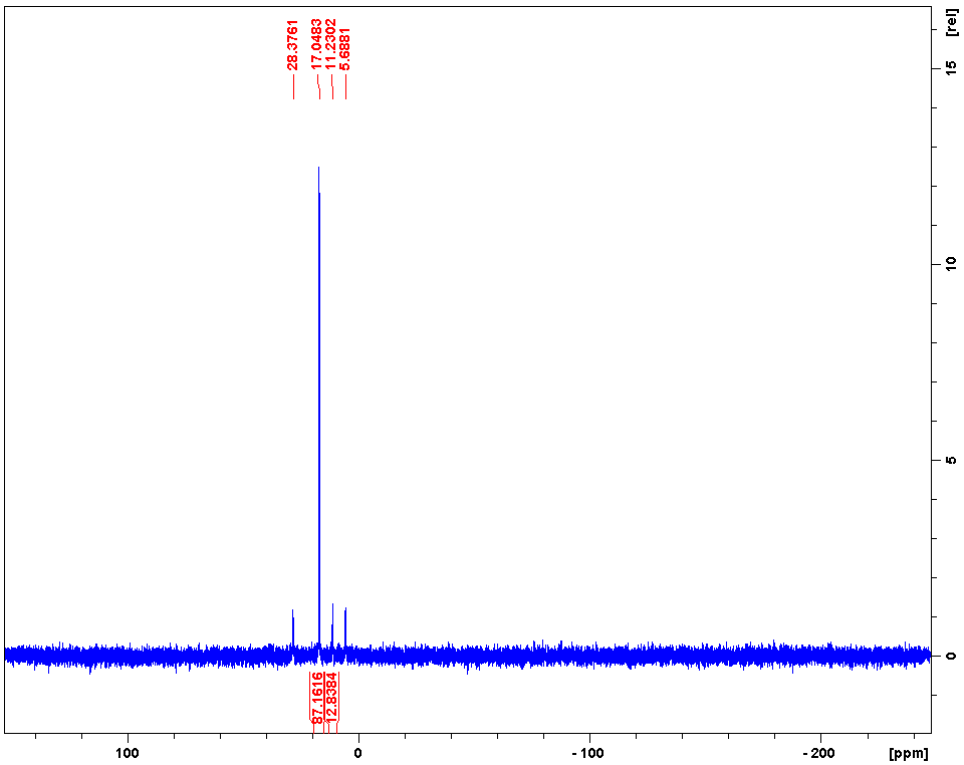
10E, 10E + 3 and 12E'

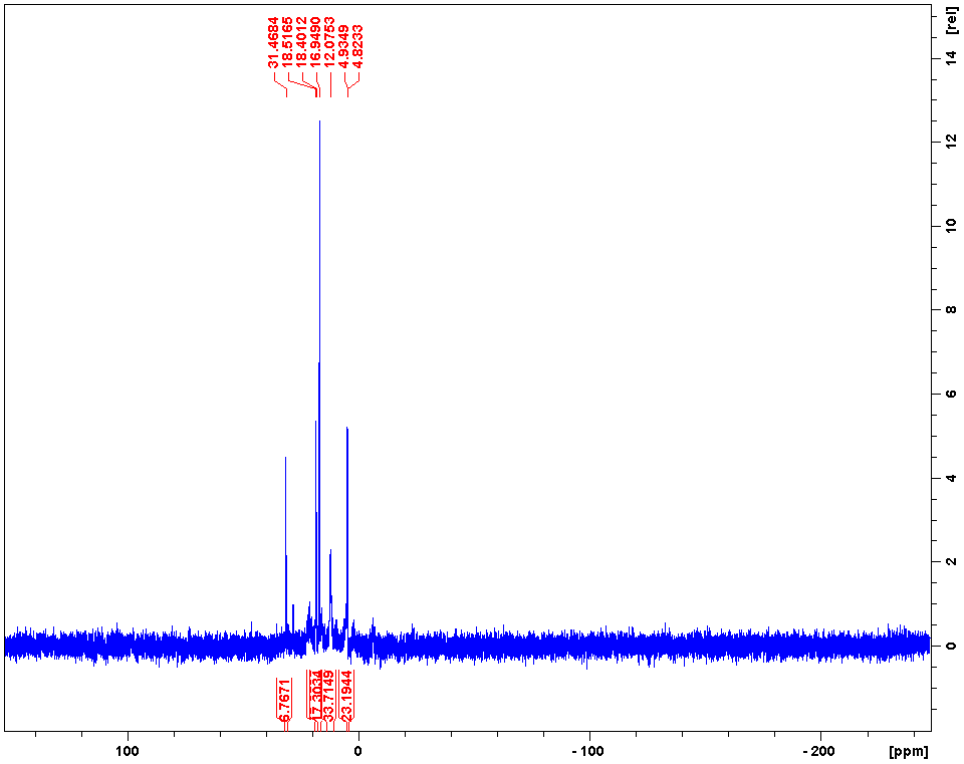
10E ^{31}P-{^{1}H}-NMR (161 MHz, CD_2Cl_2)



10E + 3 ^{31}P-{^{1}H}-NMR (161 MHz, CD_2Cl_2)



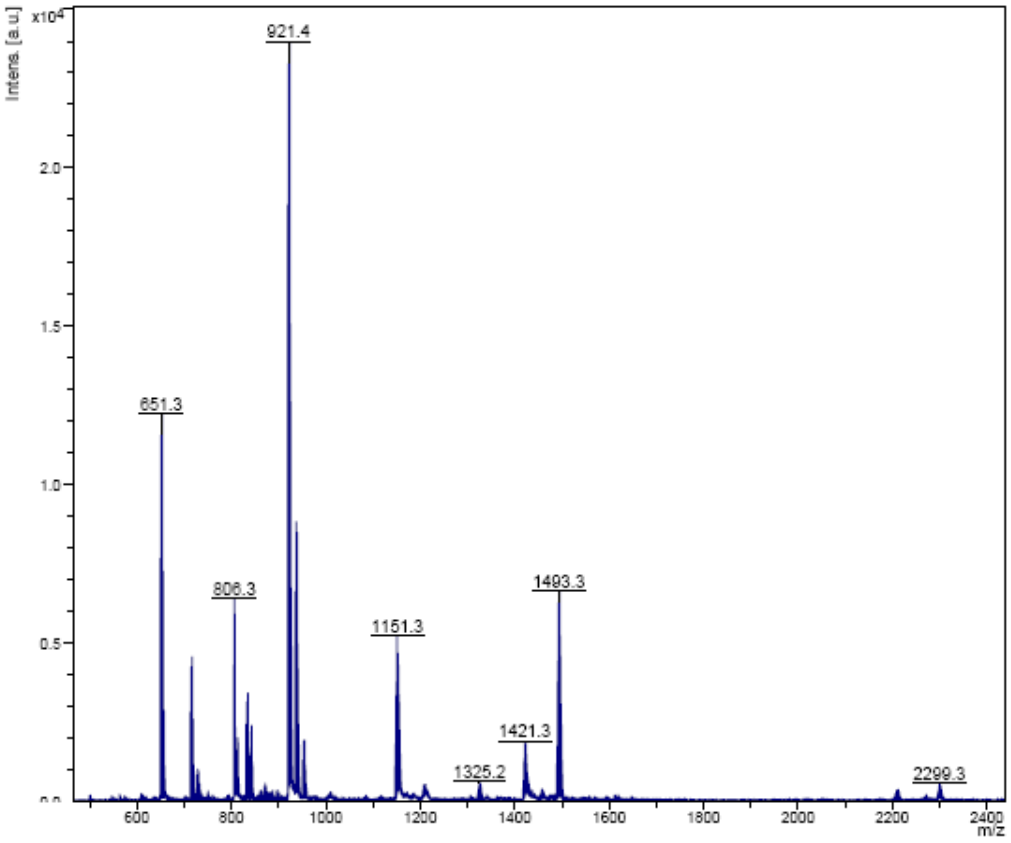
12E' ^{31}P-{^{1}H}-NMR (161 MHz, CD_2Cl_2)



MALDI-TOF-MS

Y:\data\ICIQ_080107\080128\SP243\0_D8\1

Comment 1 DCTB/CH2Cl2
Comment 2 MALDI+



Acquisition Parameter

Date of acquisition	2008-01-28 16:38:52
Acquisition method name	D:\Methods\flexControlMethods\december07\RP_Pepmix_070831-noemi.par
Spectrum type	TOF
Parent ion mass for ms/ms spectra	1000
Parent mass + PCIS upper mass limit	0
Parent mass - PCIS lower mass limit	0
CID valve/mode	false

Instrument Info

User	tof-user
Instrument	FLEX-PC
Instrument type	autoflex

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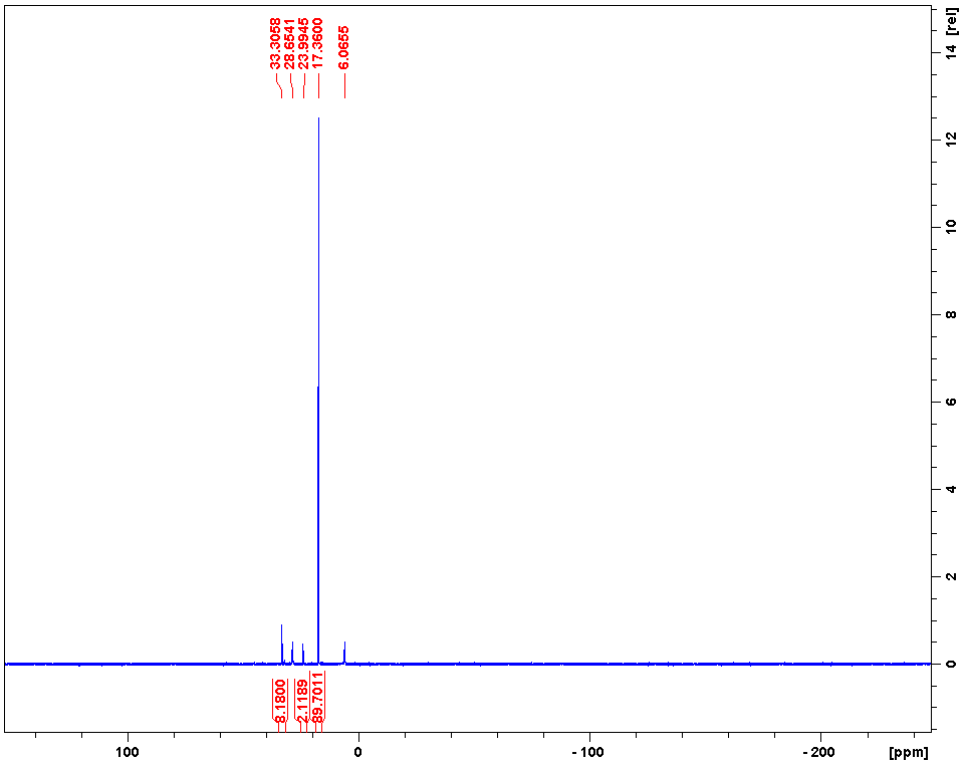
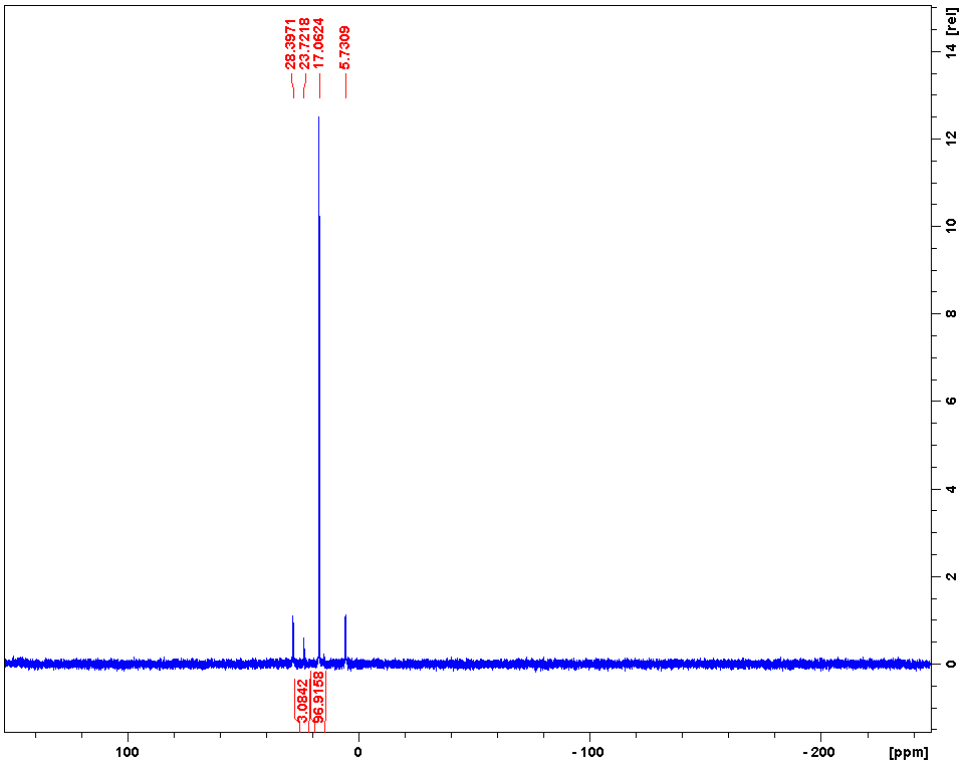
10F, 10F', 10F + 3, and 12F'

Method 1

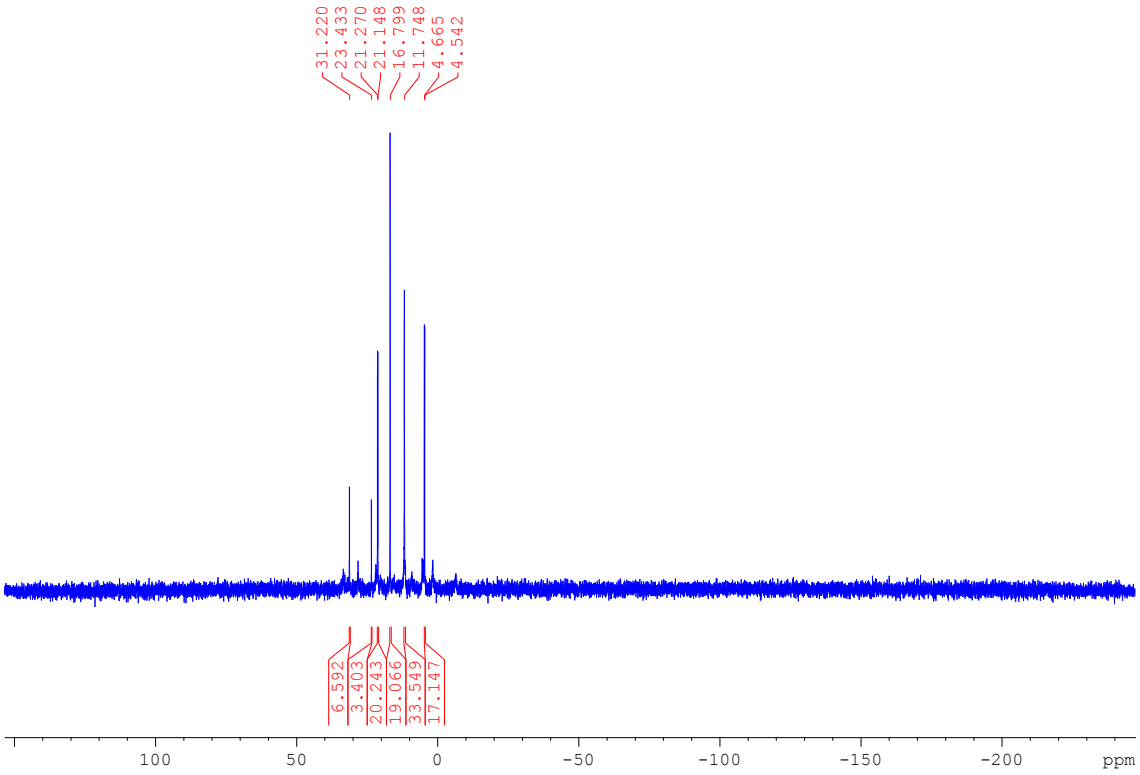
10F ^{31}P-{^{1}H}-NMR (161 MHz, CD_2Cl_2)



10F + 3 ^{31}P-{^{1}H}-NMR (161 MHz, CD_2Cl_2)

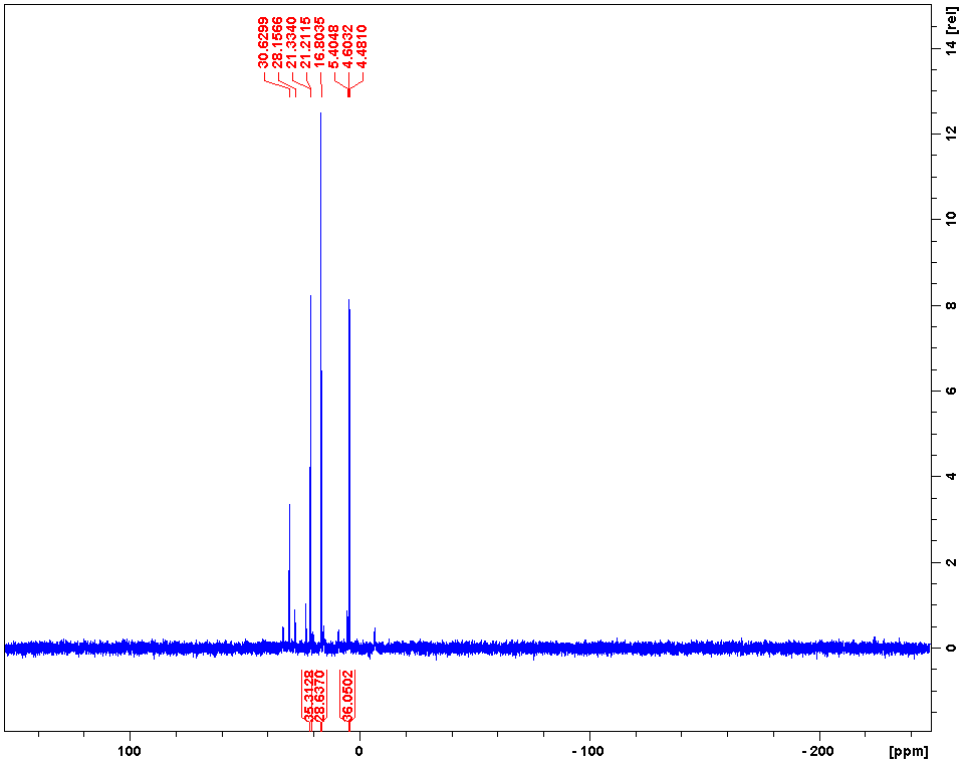


12F' ^{31}P-{^{1}H}-NMR (161 MHz, CD_2Cl_2)

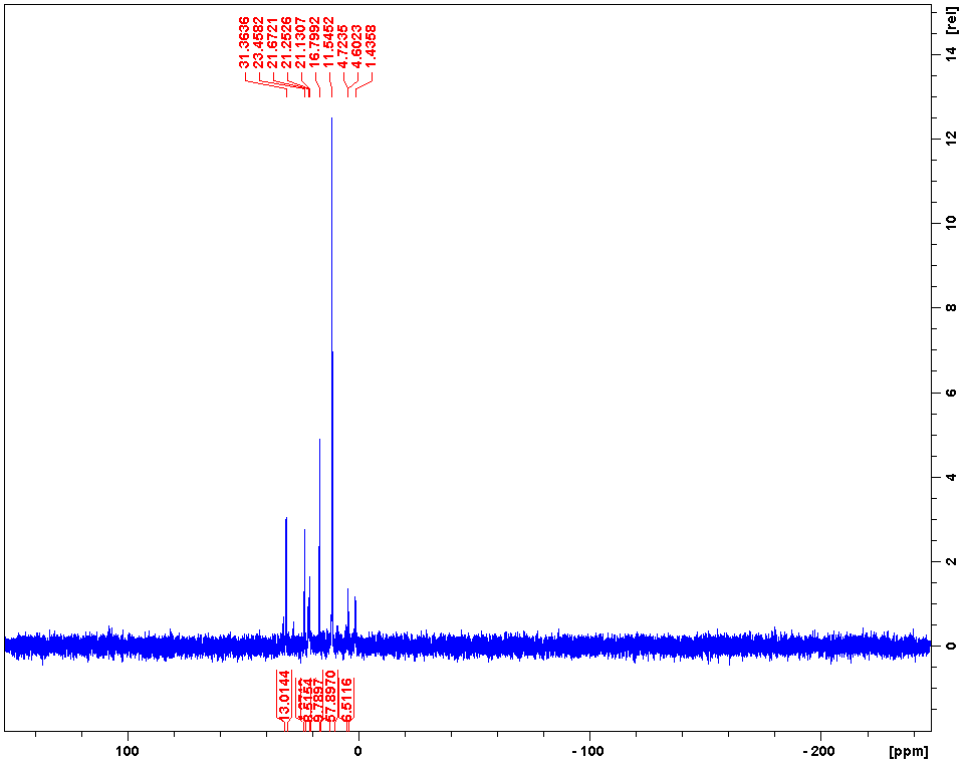


Method 2

10F + base ^{31}P-{^{1}H}-NMR (161 MHz, CD_2Cl_2)



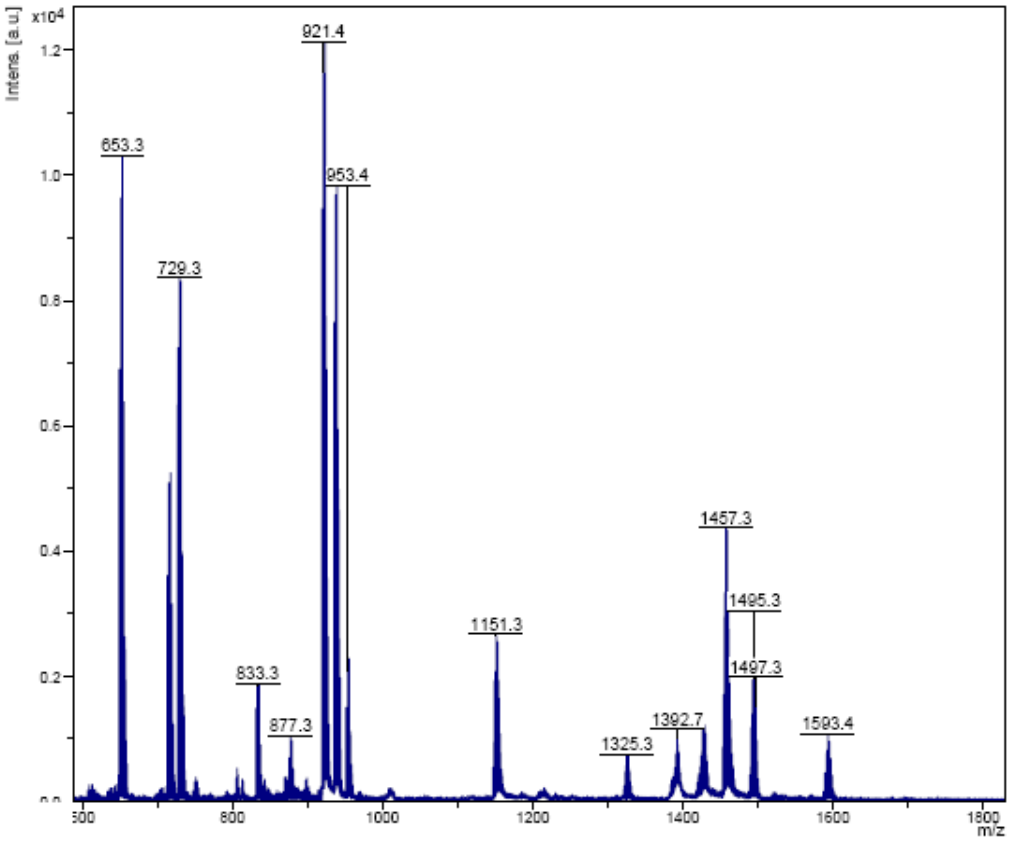
12F' ^{31}P-{^{1}H}-NMR (161 MHz, CD_2Cl_2)



MALDI-TOF-MS

Y:\data\ICIQ_080107\080128\SP245\0_D6\1

Comment 1 DCTB/CH2Cl2
Comment 2 MALDI+



Acquisition Parameter

Date of acquisition	2008-01-28 16:40:12
Acquisition method name	D:\Methods\flexControlMethods\december07\RP_Pepmix_070831-noemi.par
Spectrum type	TOF
Parent ion mass for ms/ms spectra	1000
Parent mass + PCIS upper mass limit	0
Parent mass - PCIS lower mass limit	0
CID valve/mode	false

Instrument Info

User	tof-user
Instrument	FLEX-PC
Instrument type	autoflex

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Rhodium (I) catalyzed hydroformylation of 1-octene

Conditions for the GC analyses:

Column: HP-5 Agilent Technologies; L: 30m; I.D.: 0.32mm; Film: 0.25µm
Injection Volume: 1 µl
T_{inj}: 260 ºC
Pressure:12 psi
Flow: 6 mL/min
Split: 50:1
Oven Temperature: 40 ºC, 5 min; 20 ºC/min; 150 ºC, 10 min
T_{det}: 300 ºC
Retention times (min): 4.8 (1-octene), 5.1 (4-octene), 5.3 (3-octene), 5.5 (2-octene), 8.9 (decane), 9.6 (branched aldehyde), 10.0 (linear aldehyde).