Supporting Information for

A New Route to 2-phosphanaphthalenes

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Table 1. Crystal data and structure refinement for **4**.

Identification code	mat141	
Empirical formula	C26 H15 Mo O5 P	
Formula weight	534.29	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 17.039(5) Å	α= 90°.
	b = 6.2992(13) Å	β= 97.831(6)°.
	c = 21.025(6) Å	γ = 90°.
Volume	2235.6(11) Å^3	
Z	4	
Density (calculated)	1.587 Mg/m^3	
Absorption coefficient	0.694 mm^{-1}	
F(000)	1072	
Crystal size	0.40 x 0.06 x 0.04 mm^3	
Theta range for data collection	1.45 to 33.19°.	
Index ranges	-25<=h<=25, -9<=k<=7, -31<=l<=31	
Reflections collected	30153	
Independent reflections	14325 [R(int) = 0.1104]	
Completeness to theta = 30.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9728 and 0.7686	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14325 / 1 / 595	
Goodness-of-fit on F^2	0.970	
Final R indices [I>2sigma(I)]	R1 = 0.0704, wR2 = 0.1455	
R indices (all data)	R1 = 0.1402, wR2 = 0.2063	
Absolute structure parameter	-0.07(5)	

Largest diff. peak and hole	1.186 and -1.952 e.Å^{-3}

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

	x	y	z	U(eq)
Mo(1)	3089(1)	2537(1)	5169(1)	15(1)
Mo(2)	5858(1)	3092(1)	1568(1)	16(1)
C(1)	3424(5)	-127(13)	4693(4)	18(2)
C(2)	4152(5)	3980(13)	5052(4)	20(2)
C(3)	3593(5)	1308(14)	6023(4)	22(2)
C(4)	2729(6)	5131(14)	5635(4)	26(2)
C(5)	2033(5)	1075(13)	5239(4)	19(2)
C(6)	1674(5)	5972(13)	4139(4)	18(2)
C(7)	1235(5)	6729(12)	3602(4)	17(2)
C(8)	1344(5)	5988(12)	2968(4)	16(2)
C(9)	824(5)	6657(13)	2438(4)	21(2)
C(10)	922(5)	6061(13)	1825(4)	22(2)
C(11)	1566(5)	4785(12)	1723(4)	20(2)
C(12)	2080(5)	4082(12)	2226(4)	17(2)
C(13)	1974(4)	4607(12)	2864(4)	15(2)
C(14)	2493(5)	3642(12)	3377(3)	15(2)
C(15)	628(4)	8375(13)	3696(4)	16(2)
C(16)	589(5)	10347(13)	3387(4)	21(2)
C(17)	70(5)	11900(14)	3529(4)	24(2)
C(18)	-421(5)	11515(14)	3982(5)	26(2)
C(19)	-396(5)	9599(15)	4288(4)	25(2)
C(20)	121(4)	8038(13)	4150(3)	18(2)
C(21)	3143(5)	2151(12)	3249(3)	16(2)
C(22)	2972(5)	161(13)	2976(4)	21(2)
C(23)	3575(6)	-1240(13)	2896(4)	24(2)
C(24)	4365(5)	-652(14)	3075(4)	24(2)
C(25)	4533(5)	1330(15)	3337(4)	26(2)
C(26)	3937(5)	2742(14)	3423(3)	19(2)
C(27)	5252(5)	359(13)	1297(4)	21(2)
C(28)	5523(6)	4449(14)	682(4)	26(2)
C(29)	4873(5)	4308(13)	1862(4)	19(2)

C(30)	6177(5)	1737(14)	2454(4)	19(2)
C(31)	6428(5)	5829(13)	1893(4)	21(2)
C(32)	7015(5)	-208(12)	566(4)	17(2)
C(33)	7672(5)	-980(13)	320(4)	18(2)
C(34)	8469(5)	-247(12)	541(4)	16(2)
C(35)	9118(5)	-965(13)	237(4)	19(2)
C(36)	9886(6)	-435(13)	450(4)	24(2)
C(37)	10060(5)	886(13)	1007(4)	22(2)
C(38)	9454(5)	1690(12)	1283(4)	18(2)
C(39)	8635(5)	1215(13)	1068(4)	16(2)
C(40)	8036(5)	2188(11)	1383(4)	17(2)
C(41)	7526(5)	-2651(13)	-200(4)	19(2)
C(42)	7913(5)	-4617(12)	-133(4)	18(2)
C(43)	7752(6)	-6168(13)	-603(4)	23(2)
C(44)	7205(6)	-5785(13)	-1145(4)	24(2)
C(45)	6823(5)	-3856(13)	-1199(4)	22(2)
C(46)	6975(4)	-2296(14)	-729(3)	16(2)
C(47)	8241(5)	3760(13)	1913(4)	19(2)
C(48)	8549(5)	5739(13)	1797(4)	22(2)
C(49)	8677(5)	7258(13)	2290(4)	22(2)
C(50)	8501(5)	6785(14)	2896(4)	24(2)
C(51)	8198(5)	4818(13)	3015(4)	22(2)
C(52)	8059(5)	3297(15)	2533(4)	22(2)
O(1)	3605(4)	-1639(9)	4466(3)	28(1)
O(2)	4743(4)	4747(10)	4989(4)	34(2)
O(3)	3887(5)	624(12)	6491(3)	43(2)
O(4)	2516(4)	6589(11)	5886(3)	37(2)
O(5)	1428(4)	308(10)	5275(3)	28(2)
O(6)	4922(4)	-1219(9)	1174(3)	28(2)
O(7)	5325(6)	5201(12)	204(3)	51(2)
O(8)	4310(4)	5030(10)	2019(3)	29(2)
O(9)	6334(4)	958(10)	2944(3)	28(1)
O(10)	6716(4)	7391(10)	2078(3)	30(1)
P(1)	2430(1)	4116(3)	4169(1)	16(1)
P(2)	7046(1)	1659(3)	1173(1)	17(1)

Table 3. Bond lengths [Å] and angles [°] for **4**.

Mo(1)-C(3)	2.034(9)
Mo(1)-C(4)	2.042(10)
Mo(1)-C(5)	2.043(9)
Mo(1)-C(2)	2.072(9)
Mo(1)-C(1)	2.073(8)
Mo(1)-P(1)	2.455(2)
Mo(2)-C(29)	2.017(9)
Mo(2)-C(27)	2.048(9)
Mo(2)-C(31)	2.049(9)
Mo(2)-C(30)	2.053(8)
Mo(2)-C(28)	2.058(9)
Mo(2)-P(2)	2.462(2)
C(1)-O(1)	1.127(10)
C(2)-O(2)	1.140(10)
C(3)-O(3)	1.128(11)
C(4)-O(4)	1.143(11)
C(5)-O(5)	1.150(10)
C(6)-C(7)	1.353(11)
C(6)-P(1)	1.734(8)
C(6)-H(6)	0.9500
C(7)-C(8)	1.448(11)
C(7)-C(15)	1.497(10)
C(8)-C(9)	1.391(11)
C(8)-C(13)	1.422(11)
C(9)-C(10)	1.374(12)
C(9)-H(9)	0.9500
C(10)-C(11)	1.400(12)
C(10)-H(10)	0.9500
C(11)-C(12)	1.352(11)
C(11)-H(11)	0.9500
C(12)-C(13)	1.417(11)
C(12)-H(12)	0.9500
C(13)-C(14)	1.433(10)
C(14)-C(21)	1.504(10)

C(14)-P(1)	1.710(7)
C(15)-C(20)	1.388(10)
C(15)-C(16)	1.399(11)
C(16)-C(17)	1.379(12)
C(16)-H(16)	0.9500
C(17)-C(18)	1.372(13)
C(17)-H(17)	0.9500
C(18)-C(19)	1.366(13)
C(18)-H(18)	0.9500
C(19)-C(20)	1.377(11)
C(19)-H(19)	0.9500
C(20)-H(20)	0.9500
C(21)-C(22)	1.393(11)
C(21)-C(26)	1.402(11)
C(22)-C(23)	1.382(12)
C(22)-H(22)	0.9500
C(23)-C(24)	1.398(13)
C(23)-H(23)	0.9500
C(24)-C(25)	1.379(13)
C(24)-H(24)	0.9500
C(25)-C(26)	1.381(12)
C(25)-H(25)	0.9500
C(26)-H(26)	0.9500
C(27)-O(6)	1.154(10)
C(28)-O(7)	1.121(10)
C(29)-O(8)	1.150(10)
C(30)-O(9)	1.140(10)
C(31)-O(10)	1.143(10)
C(32)-C(33)	1.385(11)
C(32)-P(2)	1.730(8)
C(32)-H(32)	0.9500
C(33)-C(34)	1.449(11)
C(33)-C(41)	1.513(11)
C(34)-C(35)	1.425(11)
C(34)-C(39)	1.439(11)
C(35)-C(36)	1.366(13)

C(35)-H(35)	0.9500
C(36)-C(37)	1.433(12)
C(36)-H(36)	0.9500
C(37)-C(38)	1.352(11)
C(37)-H(37)	0.9500
C(38)-C(39)	1.438(11)
C(38)-H(38)	0.9500
C(39)-C(40)	1.428(11)
C(40)-C(47)	1.497(11)
C(40)-P(2)	1.717(8)
C(41)-C(46)	1.373(10)
C(41)-C(42)	1.402(11)
C(42)-C(43)	1.391(11)
C(42)-H(42)	0.9500
C(43)-C(44)	1.392(12)
C(43)-H(43)	0.9500
C(44)-C(45)	1.376(12)
C(44)-H(44)	0.9500
C(45)-C(46)	1.393(11)
C(45)-H(45)	0.9500
C(46)-H(46)	0.9500
C(47)-C(48)	1.386(12)
C(47)-C(52)	1.412(11)
C(48)-C(49)	1.406(11)
C(48)-H(48)	0.9500
C(49)-C(50)	1.380(12)
C(49)-H(49)	0.9500
C(50)-C(51)	1.378(12)
C(50)-H(50)	0.9500
C(51)-C(52)	1.391(12)
C(51)-H(51)	0.9500
C(52)-H(52)	0.9500

C(3)-Mo(1)-C(4)	90.0(4)
C(3)-Mo(1)-C(5)	92.0(3)
C(4)-Mo(1)-C(5)	90.1(4)

C(3)-Mo(1)-C(2)	90.1(3)
C(4)-Mo(1)-C(2)	91.7(4)
C(5)-Mo(1)-C(2)	177.3(3)
C(3)-Mo(1)-C(1)	90.4(3)
C(4)-Mo(1)-C(1)	178.6(4)
C(5)-Mo(1)-C(1)	88.5(3)
C(2)-Mo(1)-C(1)	89.7(3)
C(3)-Mo(1)-P(1)	177.0(3)
C(4)-Mo(1)-P(1)	87.4(3)
C(5)-Mo(1)-P(1)	86.6(2)
C(2)-Mo(1)-P(1)	91.5(2)
C(1)-Mo(1)-P(1)	92.2(2)
C(29)-Mo(2)-C(27)	89.8(3)
C(29)-Mo(2)-C(31)	87.4(3)
C(27)-Mo(2)-C(31)	176.2(4)
C(29)-Mo(2)-C(30)	90.5(3)
C(27)-Mo(2)-C(30)	88.0(3)
C(31)-Mo(2)-C(30)	89.6(3)
C(29)-Mo(2)-C(28)	88.9(4)
C(27)-Mo(2)-C(28)	91.7(4)
C(31)-Mo(2)-C(28)	90.7(3)
C(30)-Mo(2)-C(28)	179.2(4)
C(29)-Mo(2)-P(2)	178.0(2)
C(27)-Mo(2)-P(2)	90.2(2)
C(31)-Mo(2)-P(2)	92.7(3)
C(30)-Mo(2)-P(2)	91.5(2)
C(28)-Mo(2)-P(2)	89.2(3)
O(1)-C(1)-Mo(1)	176.0(7)
O(2)-C(2)-Mo(1)	179.0(7)
O(3)-C(3)-Mo(1)	178.5(9)
O(4)-C(4)-Mo(1)	178.6(8)
O(5)-C(5)-Mo(1)	178.0(7)
C(7)-C(6)-P(1)	126.3(6)
C(7)-C(6)-H(6)	116.9
P(1)-C(6)-H(6)	116.9
C(6)-C(7)-C(8)	121.9(7)

C(6)-C(7)-C(15)	116.6(7)
C(8)-C(7)-C(15)	121.5(7)
C(9)-C(8)-C(13)	118.3(8)
C(9)-C(8)-C(7)	119.5(7)
C(13)-C(8)-C(7)	122.3(7)
C(10)-C(9)-C(8)	121.6(8)
C(10)-C(9)-H(9)	119.2
C(8)-C(9)-H(9)	119.2
C(9)-C(10)-C(11)	119.9(8)
C(9)-C(10)-H(10)	120.0
C(11)-C(10)-H(10)	120.0
C(12)-C(11)-C(10)	120.4(8)
C(12)-C(11)-H(11)	119.8
C(10)-C(11)-H(11)	119.8
C(11)-C(12)-C(13)	120.8(8)
C(11)-C(12)-H(12)	119.6
C(13)-C(12)-H(12)	119.6
C(12)-C(13)-C(8)	119.0(7)
C(12)-C(13)-C(14)	117.9(7)
C(8)-C(13)-C(14)	123.0(7)
C(13)-C(14)-C(21)	121.6(6)
C(13)-C(14)-P(1)	123.0(6)
C(21)-C(14)-P(1)	115.4(5)
C(20)-C(15)-C(16)	117.5(7)
C(20)-C(15)-C(7)	119.4(7)
C(16)-C(15)-C(7)	122.9(7)
C(17)-C(16)-C(15)	121.3(8)
C(17)-C(16)-H(16)	119.3
C(15)-C(16)-H(16)	119.3
C(18)-C(17)-C(16)	119.6(8)
C(18)-C(17)-H(17)	120.2
C(16)-C(17)-H(17)	120.2
C(19)-C(18)-C(17)	120.0(8)
C(19)-C(18)-H(18)	120.0
C(17)-C(18)-H(18)	120.0
C(18)-C(19)-C(20)	120.7(9)

C(18)-C(19)-H(19)	119.6
C(20)-C(19)-H(19)	119.6
C(19)-C(20)-C(15)	120.8(8)
C(19)-C(20)-H(20)	119.6
C(15)-C(20)-H(20)	119.6
C(22)-C(21)-C(26)	119.1(7)
C(22)-C(21)-C(14)	121.2(7)
C(26)-C(21)-C(14)	119.7(7)
C(23)-C(22)-C(21)	120.5(8)
C(23)-C(22)-H(22)	119.7
C(21)-C(22)-H(22)	119.7
C(22)-C(23)-C(24)	120.2(8)
C(22)-C(23)-H(23)	119.9
C(24)-C(23)-H(23)	119.9
C(25)-C(24)-C(23)	119.1(8)
C(25)-C(24)-H(24)	120.4
C(23)-C(24)-H(24)	120.4
C(24)-C(25)-C(26)	121.3(8)
C(24)-C(25)-H(25)	119.4
C(26)-C(25)-H(25)	119.4
C(25)-C(26)-C(21)	119.7(8)
C(25)-C(26)-H(26)	120.1
C(21)-C(26)-H(26)	120.1
O(6)-C(27)-Mo(2)	176.6(7)
O(7)-C(28)-Mo(2)	178.5(10)
O(8)-C(29)-Mo(2)	178.6(8)
O(9)-C(30)-Mo(2)	178.1(7)
O(10)-C(31)-Mo(2)	177.1(8)
C(33)-C(32)-P(2)	124.7(7)
C(33)-C(32)-H(32)	117.6
P(2)-C(32)-H(32)	117.6
C(32)-C(33)-C(34)	122.5(7)
C(32)-C(33)-C(41)	116.9(7)
C(34)-C(33)-C(41)	120.6(7)
C(35)-C(34)-C(39)	117.8(7)
C(35)-C(34)-C(33)	120.3(7)

C(39)-C(34)-C(33)	121.9(7)
C(36)-C(35)-C(34)	122.8(8)
C(36)-C(35)-H(35)	118.6
C(34)-C(35)-H(35)	118.6
C(35)-C(36)-C(37)	119.5(8)
C(35)-C(36)-H(36)	120.2
C(37)-C(36)-H(36)	120.2
C(38)-C(37)-C(36)	118.9(8)
C(38)-C(37)-H(37)	120.6
C(36)-C(37)-H(37)	120.6
C(37)-C(38)-C(39)	123.5(8)
C(37)-C(38)-H(38)	118.2
C(39)-C(38)-H(38)	118.2
C(40)-C(39)-C(38)	119.3(7)
C(40)-C(39)-C(34)	123.6(7)
C(38)-C(39)-C(34)	117.1(7)
C(39)-C(40)-C(47)	121.3(7)
C(39)-C(40)-P(2)	122.5(6)
C(47)-C(40)-P(2)	116.3(6)
C(46)-C(41)-C(42)	119.1(7)
C(46)-C(41)-C(33)	120.0(7)
C(42)-C(41)-C(33)	120.9(7)
C(43)-C(42)-C(41)	120.3(8)
C(43)-C(42)-H(42)	119.9
C(41)-C(42)-H(42)	119.9
C(42)-C(43)-C(44)	120.4(8)
C(42)-C(43)-H(43)	119.8
C(44)-C(43)-H(43)	119.8
C(45)-C(44)-C(43)	118.5(8)
C(45)-C(44)-H(44)	120.7
C(43)-C(44)-H(44)	120.7
C(44)-C(45)-C(46)	121.6(8)
C(44)-C(45)-H(45)	119.2
C(46)-C(45)-H(45)	119.2
C(41)-C(46)-C(45)	120.1(8)
C(41)-C(46)-H(46)	120.0

C(45)-C(46)-H(46)	120.0
C(48)-C(47)-C(52)	118.9(8)
C(48)-C(47)-C(40)	121.3(7)
C(52)-C(47)-C(40)	119.5(7)
C(47)-C(48)-C(49)	120.5(8)
C(47)-C(48)-H(48)	119.8
C(49)-C(48)-H(48)	119.8
C(50)-C(49)-C(48)	120.1(8)
C(50)-C(49)-H(49)	119.9
C(48)-C(49)-H(49)	119.9
C(51)-C(50)-C(49)	119.7(8)
C(51)-C(50)-H(50)	120.2
C(49)-C(50)-H(50)	120.2
C(50)-C(51)-C(52)	121.3(8)
C(50)-C(51)-H(51)	119.4
C(52)-C(51)-H(51)	119.4
C(51)-C(52)-C(47)	119.5(8)
C(51)-C(52)-H(52)	120.2
C(47)-C(52)-H(52)	120.2
C(14)-P(1)-C(6)	103.2(4)
C(14)-P(1)-Mo(1)	132.9(3)
C(6)-P(1)-Mo(1)	123.7(3)
C(40)-P(2)-C(32)	104.6(4)
C(40)-P(2)-Mo(2)	131.7(3)
C(32)-P(2)-Mo(2)	123.7(3)

Symmetry transformations used to generate equivalent atoms:

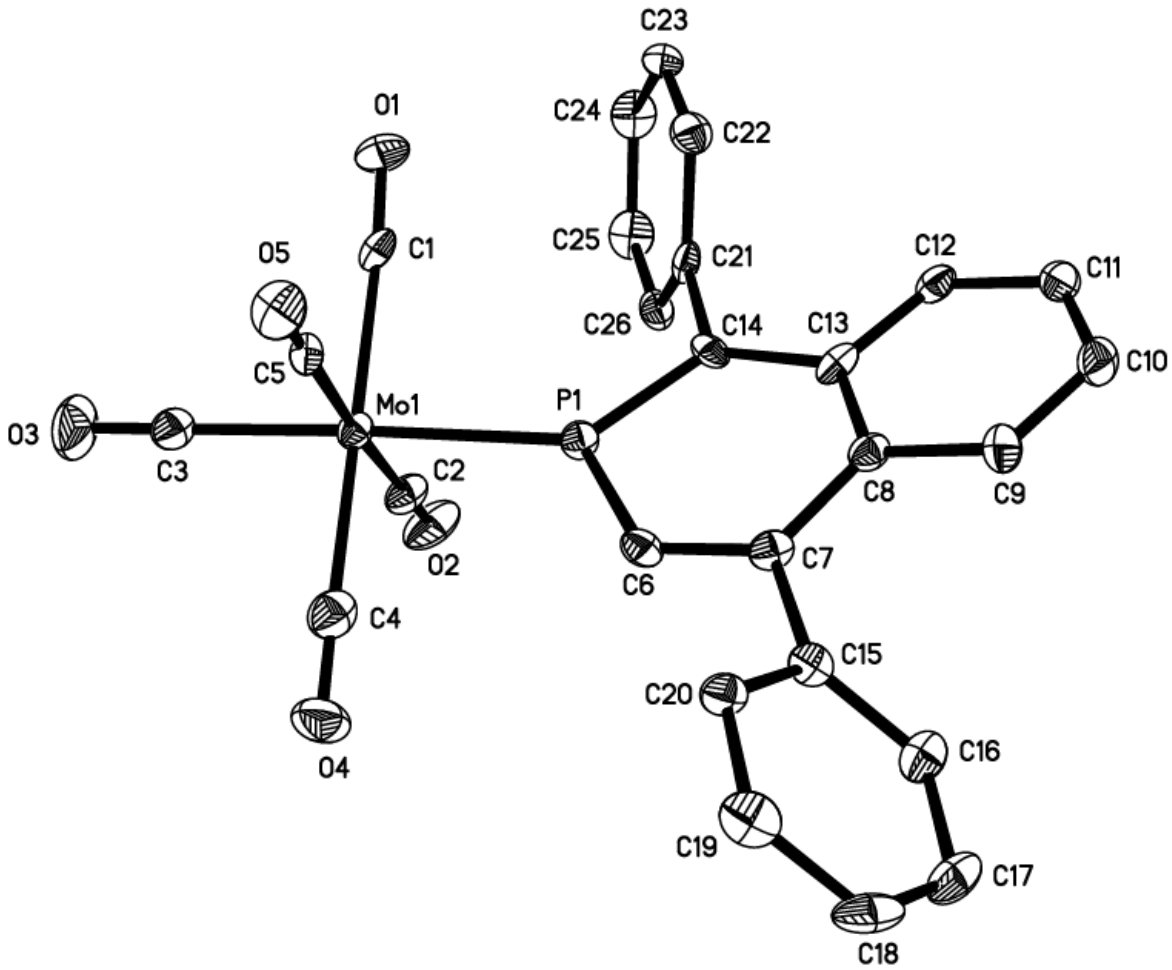
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

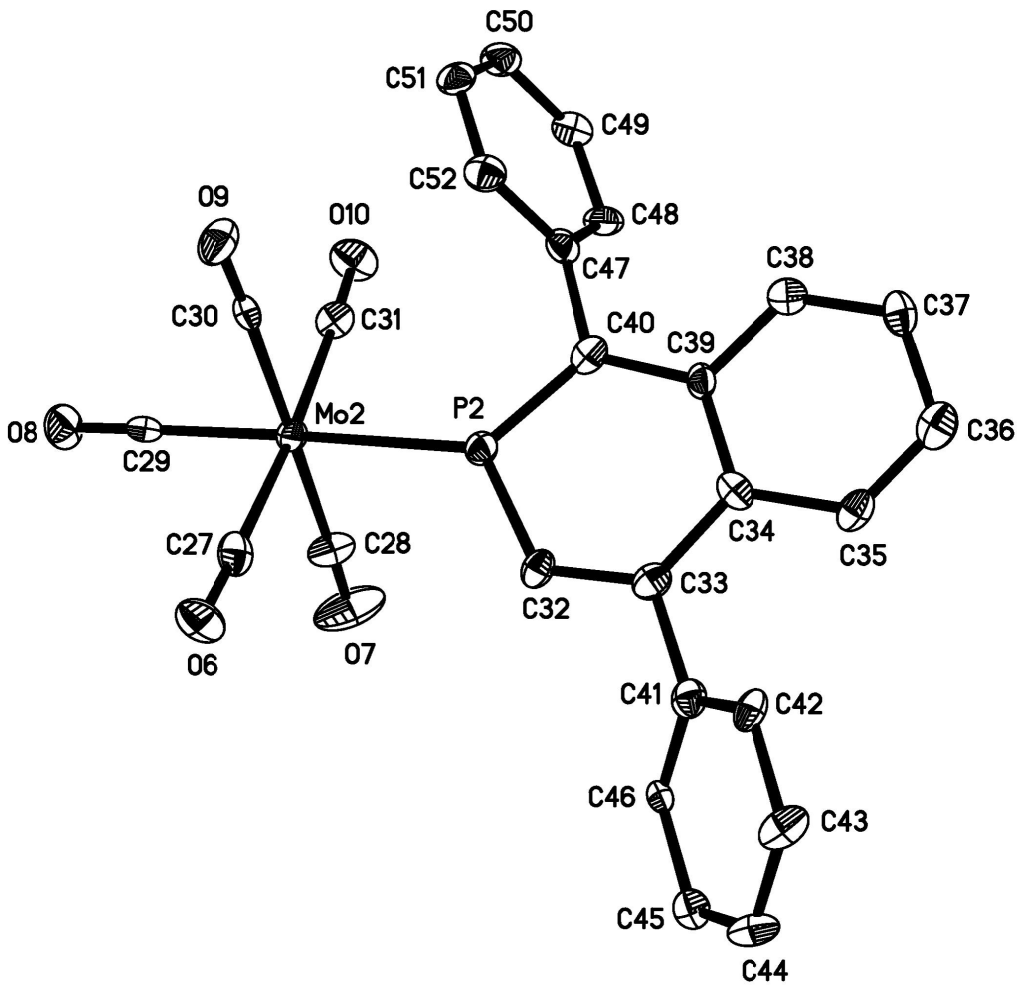
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	14(1)	15(1)	17(1)	2(1)	0(1)	0(1)
Mo(2)	15(1)	16(1)	16(1)	-2(1)	3(1)	2(1)
C(1)	19(4)	14(4)	23(4)	7(3)	3(3)	3(3)
C(2)	15(4)	17(4)	28(4)	4(3)	-3(3)	4(3)
C(3)	22(5)	19(4)	24(4)	0(3)	2(4)	-1(3)
C(4)	25(5)	24(5)	30(5)	2(4)	-1(4)	-1(4)
C(5)	28(5)	17(4)	13(4)	3(3)	3(3)	2(3)
C(6)	22(4)	19(4)	15(4)	-4(3)	6(3)	1(3)
C(7)	12(4)	15(4)	22(4)	-1(3)	1(3)	1(3)
C(8)	14(4)	13(4)	21(4)	1(3)	0(3)	1(3)
C(9)	21(4)	23(4)	18(4)	2(3)	-2(3)	2(3)
C(10)	19(4)	22(4)	23(4)	2(3)	-7(3)	0(3)
C(11)	29(5)	17(4)	16(4)	2(3)	6(3)	-7(3)
C(12)	20(4)	13(4)	20(4)	3(3)	7(3)	4(3)
C(13)	8(3)	12(4)	26(4)	6(3)	4(3)	0(3)
C(14)	14(4)	17(4)	13(3)	-4(3)	1(3)	-5(3)
C(15)	10(3)	20(4)	18(3)	-2(3)	1(3)	2(3)
C(16)	17(4)	20(4)	26(4)	4(3)	1(3)	-2(3)
C(17)	18(4)	17(4)	36(5)	5(3)	-2(4)	3(3)
C(18)	17(4)	16(4)	43(5)	-12(4)	-1(4)	-1(3)
C(19)	18(4)	30(5)	28(5)	-4(4)	5(4)	0(4)
C(20)	14(3)	17(4)	20(3)	-2(3)	-1(3)	4(3)
C(21)	18(4)	17(4)	14(3)	7(3)	4(3)	7(3)
C(22)	18(4)	22(4)	21(4)	-1(3)	-1(3)	-1(3)
C(23)	37(5)	16(4)	18(4)	-4(3)	3(4)	3(3)
C(24)	17(4)	29(5)	27(4)	0(4)	10(3)	16(3)
C(25)	19(4)	32(5)	28(5)	2(4)	6(4)	2(4)
C(26)	22(4)	22(4)	14(3)	0(3)	3(3)	1(3)
C(27)	17(4)	20(4)	25(4)	4(3)	5(3)	6(3)
C(28)	37(6)	22(5)	17(4)	-2(3)	-1(4)	4(4)
C(29)	18(4)	22(4)	15(4)	-4(3)	-2(3)	-3(3)

C(30)	9(4)	29(4)	20(4)	-3(3)	3(3)	0(3)
C(31)	26(5)	18(4)	21(4)	0(3)	4(3)	0(3)
C(32)	21(4)	13(4)	18(4)	-1(3)	7(3)	2(3)
C(33)	23(4)	17(4)	16(4)	1(3)	3(3)	1(3)
C(34)	15(4)	14(4)	20(4)	8(3)	0(3)	-2(3)
C(35)	27(5)	11(4)	21(4)	-2(3)	10(3)	-1(3)
C(36)	30(5)	19(4)	25(4)	4(3)	11(4)	-2(4)
C(37)	17(4)	23(4)	27(4)	4(3)	7(3)	0(3)
C(38)	22(4)	11(4)	21(4)	0(3)	2(3)	-2(3)
C(39)	13(4)	17(4)	19(4)	-1(3)	6(3)	-2(3)
C(40)	26(4)	10(4)	18(4)	0(3)	8(3)	-4(3)
C(41)	19(4)	20(4)	19(3)	1(3)	7(3)	-4(3)
C(42)	22(4)	20(4)	14(4)	3(3)	8(3)	3(3)
C(43)	38(5)	14(4)	18(4)	0(3)	8(4)	-2(4)
C(44)	34(5)	20(4)	17(4)	-5(3)	-1(4)	-5(4)
C(45)	17(4)	25(4)	22(4)	-1(3)	3(3)	0(3)
C(46)	9(3)	20(4)	19(3)	-5(3)	3(3)	-2(3)
C(47)	14(4)	22(4)	20(4)	2(3)	0(3)	3(3)
C(48)	22(4)	27(5)	16(4)	-1(3)	-2(3)	-4(4)
C(49)	24(4)	16(4)	24(4)	0(3)	-2(3)	1(3)
C(50)	24(5)	24(4)	23(4)	-8(3)	-1(4)	2(3)
C(51)	23(4)	28(5)	13(4)	2(3)	0(3)	7(3)
C(52)	24(4)	21(4)	20(4)	3(3)	0(3)	-1(4)
O(1)	30(3)	16(3)	37(3)	-4(3)	7(3)	6(3)
O(2)	23(4)	21(3)	55(5)	8(3)	-4(3)	-8(3)
O(3)	49(5)	44(5)	30(4)	12(3)	-14(4)	-5(4)
O(4)	45(4)	31(4)	31(4)	-10(3)	-5(3)	17(3)
O(5)	23(3)	32(4)	32(4)	3(3)	13(3)	-11(3)
O(6)	27(4)	17(3)	39(4)	-4(3)	-1(3)	-5(3)
O(7)	92(7)	38(4)	20(4)	2(3)	-4(4)	17(4)
O(8)	23(3)	26(3)	38(4)	-9(3)	9(3)	4(3)
O(9)	31(4)	33(4)	21(3)	4(3)	9(3)	3(3)
O(10)	32(3)	18(3)	39(3)	-6(3)	-1(3)	-1(3)
P(1)	14(1)	16(1)	16(1)	0(1)	2(1)	2(1)
P(2)	17(1)	16(1)	18(1)	-3(1)	4(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4**.

	x	y	z	U(eq)
H(6)	1557	6509	4538	22
H(9)	392	7548	2501	25
H(10)	553	6513	1472	27
H(11)	1642	4412	1298	25
H(12)	2517	3226	2150	21
H(16)	928	10622	3073	26
H(17)	51	13229	3314	29
H(18)	-779	12582	4083	31
H(19)	-739	9341	4601	30
H(20)	130	6714	4367	21
H(22)	2437	-236	2843	25
H(23)	3452	-2606	2718	29
H(24)	4782	-1607	3017	28
H(25)	5070	1733	3460	31
H(26)	4063	4107	3600	23
H(32)	6510	-742	390	21
H(35)	9012	-1851	-131	23
H(36)	10302	-939	232	29
H(37)	10593	1192	1178	26
H(38)	9575	2618	1639	22
H(42)	8288	-4891	236	21
H(43)	8017	-7497	-554	28
H(44)	7099	-6832	-1471	29
H(45)	6446	-3583	-1566	26
H(46)	6698	-984	-776	19
H(48)	8673	6071	1382	26
H(49)	8886	8612	2206	26
H(50)	8588	7811	3229	29
H(51)	8083	4495	3434	26
H(52)	7842	1956	2621	26


C23
O1
C24
C22
C25
C1
C21
C12
C11
O5
C26
C14
C13
C10
C5
Mo1
P1
O3
C3
C2
C8
C9
O2
C7
C6
C4
C15
C20
C16
C19
C17
C18
O4


C50
C51
C49
C52
C48
O9
O10
C47
C38
C30
C31
C40
C39
C37
Mo2
P2
O8
C29
C36
C34
C27
C28
C35
C33
C32
O6
O7
C41
C42
C46
C43
C45
C44