Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting information for

A detailed kinetic analysis of rhodium-catalyzed alkyne hydrogenation

Jingwei Luo,[a] Allen G. Oliver[b] and J. Scott McIndoe*[a]

a. Department of Chemistry, University of Victoria, P.O. Box 3065 Victoria, BC V8W3V6, Canada. Fax: +1 (250) 721-7147; Tel: +1 (250) 721-7181; E-mail: mcindoe@uvic.ca

b. Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN 46556, USA.

Numerical modeling

Rate constants for the reaction at different temperatures

Table S1. Rate constants for the reaction at 23^{o}C

Rate constant, *k*	Rate constant, *k* for forward reaction	Rate constant, *k* for back reaction
A → B	0.00385	13.6
A → F	0.0001	0.00000001
F → C	0.0033	13.6
B → C	4000	1
C → D	47	5000
C → D’	141	4000
D → E	10000	0
E → B	10000	0
D’ → E’	10000	0
E’ → B	10000	0

Table S2. Rate constants for the reaction at 58^{o}C

Rate constant, *k*	Rate constant, *k* for forward reaction	Rate constant, *k* for back reaction
A → B	0.16	15

A → F	0.0001	2.1×10^{-8}
F → C	0.155	15
B → C	4000	1
C → D	51	5000
C → D’	153	4000
D → E	10000	0
E → B	10000	0
D’ → E’	10000	0
E’ → B	10000	0

Table S3. Rate constants for the reaction at 91^{o}C

Rate constant, *k*	Rate constant, *k* for forward reaction	Rate constant, *k* for back reaction
A → B	1.8	80
A → F	0.001	0.0000002
F → C	1.8	80
B → C	8000	1
C → D	90	5000
C → D’	250	4000
D → E	10000	0

E → B	10000	0
D’ → E’	10000	0
E’ → B	10000	0

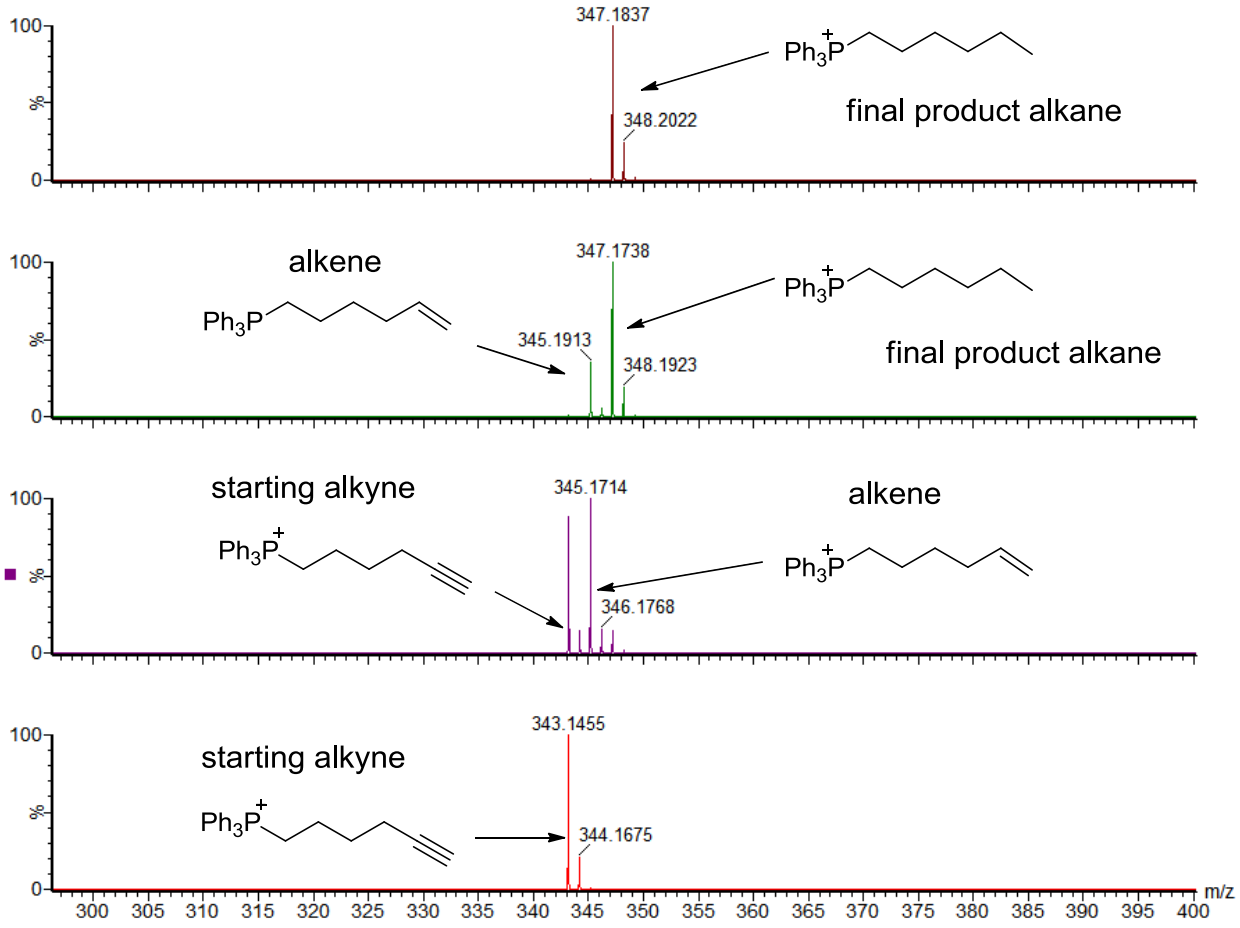


Figure S1. Positive-ion ESI-MS in fluorobenzene, $[PPh_3P(CH_2)_4CCH]PF_6$ (bottom) is the starting material. $[PPh_3P(CH_2)_5CH_3]PF_6$ (top) is the final product. The middle two spectra are snapshots during the reaction.

Table S4. Crystal data and structure refinement for $PPh_3P(CH_2)_4CCH$.

Identification code	uvic1304
Empirical formula	$C_{24}H_{24}IP$

Formula weight	470.30
Temperature	120(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 13.0516(10) Å α = 90°
	b = 12.5831(10) Å β = 96.207(4)°
	c = 13.2499(10) Å γ = 90°
Volume	2163.3(3) $Å^3$
Z	4
Density (calculated)	1.444 $g.cm^{-3}$
Absorption coefficient (μ)	1.559 mm^{-1}
F(000)	944
Crystal color, habit	colorless, rod
Crystal size	0.150 × 0.101 × 0.061 mm^3
θ range for data collection	2.081 to 28.365°
Index ranges	$-17 \leq h \leq 17$, $-15 \leq k \leq 16$, $-17 \leq l \leq 17$
Reflections collected	35698
Independent reflections	5405 [R_{int} = 0.0344]
Completeness to θ = 25.242°	100.0 %
Absorption correction	Numerical
Max. and min. transmission	0.9981 and 0.8813
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5405 / 0 / 235
Goodness-of-fit on F^2	1.015
Final R indices [I>2σ(I)]	R_1 = 0.0236, wR_2 = 0.0521
R indices (all data)	R_1 = 0.0335, wR_2 = 0.0559
Extinction coefficient	n/a
Largest diff. peak and hole	0.656 and -0.310 $e^-.Å^{-3}$

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$)

for uvic1304_x. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
P(1)	0.59437(4)	0.35145(4)	0.77633(4)	0.015(1)
C(1)	0.58625(15)	0.34134(15)	0.91035(15)	0.019(1)
C(2)	0.65005(16)	0.24609(16)	0.95519(15)	0.022(1)
C(3)	0.64279(18)	0.23386(18)	1.06805(16)	0.028(1)
C(4)	0.71426(18)	0.14714(18)	1.11623(17)	0.031(1)
C(5)	0.69245(18)	0.0405(2)	1.07102(18)	0.035(1)
C(6)	0.67377(19)	-0.0383(2)	1.03465(18)	0.035(1)
C(7)	0.72855(14)	0.35328(14)	0.75839(14)	0.016(1)
C(8)	0.78310(15)	0.44387(16)	0.79383(16)	0.023(1)
C(9)	0.88741(16)	0.45062(17)	0.78475(17)	0.028(1)
C(10)	0.93784(16)	0.36803(18)	0.74190(17)	0.028(1)
C(11)	0.88443(16)	0.27791(17)	0.70810(17)	0.026(1)
C(12)	0.77930(15)	0.27011(15)	0.71609(15)	0.020(1)
C(13)	0.53804(14)	0.47189(14)	0.72400(14)	0.017(1)
C(14)	0.44746(14)	0.51100(15)	0.75743(15)	0.020(1)
C(15)	0.39882(15)	0.59753(16)	0.70789(15)	0.022(1)
C(16)	0.43910(16)	0.64432(16)	0.62686(16)	0.023(1)
C(17)	0.52931(16)	0.60550(16)	0.59386(16)	0.025(1)
C(18)	0.57886(15)	0.51915(16)	0.64136(15)	0.022(1)
C(19)	0.52645(14)	0.24431(14)	0.70879(14)	0.017(1)
C(20)	0.54421(15)	0.22521(15)	0.60839(15)	0.021(1)
C(21)	0.48296(18)	0.15309(16)	0.55023(17)	0.026(1)
C(22)	0.40499(15)	0.09917(16)	0.59120(17)	0.026(1)
C(23)	0.38776(15)	0.11668(16)	0.69143(18)	0.027(1)
C(24)	0.44817(14)	0.18958(16)	0.75110(16)	0.022(1)
I(1)	0.78749(2)	0.13419(2)	0.45604(2)	0.022(1)
H(1A)	0.6124	0.4076	0.9442	0.023

H(1B)	0.5133	0.3323	0.9229	0.023
H(2A)	0.6249	0.1803	0.9197	0.027
H(2B)	0.7231	0.2561	0.9436	0.027
H(3A)	0.5708	0.2165	1.0789	0.034
H(3B)	0.6607	0.3024	1.1023	0.034
H(4A)	0.7865	0.1666	1.1084	0.037
H(4B)	0.7072	0.1437	1.1898	0.037
H(6)	0.6579	-0.1053	1.0037	0.042
H(8)	0.7488	0.5003	0.8239	0.027
H(9)	0.9247	0.5123	0.8081	0.033
H(10)	1.0095	0.3734	0.7357	0.034
H(11)	0.9195	0.2212	0.6793	0.031
H(12)	0.7424	0.2082	0.6927	0.024
H(14)	0.4195	0.4789	0.8133	0.024
H(15)	0.3372	0.6247	0.7301	0.026
H(16)	0.4050	0.7033	0.5935	0.028
H(17)	0.5571	0.6385	0.5383	0.030
H(18)	0.6401	0.4920	0.6182	0.026
H(20)	0.5981	0.2615	0.5800	0.026
H(21)	0.4947	0.1407	0.4817	0.032
H(22)	0.3632	0.0501	0.5508	0.032
H(23)	0.3346	0.0789	0.7196	0.032
H(24)	0.4362	0.2018	0.8196	0.027

Table 3. Anisotropic displacement parameters ($Å^2$) for uvic1304_x.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P(1)	0.0150(2)	0.0133(2)	0.0165(2)	0.0010(2)	0.0023(2)	0.0000(2)
C(1)	0.0210(9)	0.0210(9)	0.0165(9)	0.0014(7)	0.0043(7)	0.0017(7)
C(2)	0.0242(10)	0.0256(10)	0.0179(10)	0.0034(8)	0.0039(8)	0.0046(8)
C(3)	0.0340(12)	0.0317(11)	0.0191(10)	0.0019(9)	0.0034(9)	0.0039(9)
C(4)	0.0361(12)	0.0358(13)	0.0199(10)	0.0072(9)	-0.0042(9)	0.0023(10)
C(5)	0.0318(12)	0.0425(14)	0.0300(12)	0.0176(11)	-0.0017(10)	0.0068(11)
C(6)	0.0385(13)	0.0339(13)	0.0309(13)	0.0076(10)	-0.0079(10)	-0.0082(11)
C(7)	0.0139(8)	0.0172(9)	0.0164(9)	0.0002(7)	0.0011(7)	-0.0010(7)
C(8)	0.0226(10)	0.0191(9)	0.0267(11)	-0.0056(8)	0.0018(8)	-0.0001(8)
C(9)	0.0233(10)	0.0249(10)	0.0342(12)	-0.0044(9)	0.0001(9)	-0.0084(8)
C(10)	0.0149(9)	0.0399(12)	0.0301(11)	-0.0018(10)	0.0037(8)	-0.0028(9)
C(11)	0.0217(10)	0.0266(11)	0.0290(11)	-0.0045(9)	0.0034(8)	0.0047(8)
C(12)	0.0200(9)	0.0186(9)	0.0217(10)	-0.0034(7)	0.0011(8)	-0.0001(7)
C(13)	0.0170(9)	0.0135(8)	0.0189(9)	-0.0001(7)	0.0006(7)	0.0002(7)
C(14)	0.0195(9)	0.0199(9)	0.0220(10)	0.0020(8)	0.0048(8)	-0.0005(8)
C(15)	0.0193(9)	0.0225(9)	0.0243(10)	-0.0007(8)	0.0029(8)	0.0036(8)
C(16)	0.0260(10)	0.0191(10)	0.0241(10)	0.0024(8)	-0.0013(8)	0.0049(8)
C(17)	0.0302(11)	0.0227(10)	0.0224(10)	0.0054(8)	0.0069(8)	0.0035(8)
C(18)	0.0220(10)	0.0215(10)	0.0225(10)	0.0009(8)	0.0058(8)	0.0031(8)
C(19)	0.0159(9)	0.0137(8)	0.0216(10)	0.0007(7)	-0.0012(7)	0.0002(7)
C(20)	0.0247(10)	0.0181(9)	0.0202(10)	0.0029(7)	-0.0012(8)	-0.0053(8)
C(21)	0.0354(12)	0.0191(10)	0.0230(11)	0.0023(8)	-0.0062(9)	-0.0023(8)
C(22)	0.0206(10)	0.0175(9)	0.0381(12)	-0.0006(9)	-0.0085(9)	-0.0006(8)
C(23)	0.0146(9)	0.0181(10)	0.0476(14)	0.0015(9)	0.0053(9)	-0.0015(7)
C(24)	0.0166(9)	0.0195(10)	0.0321(11)	-0.0003(8)	0.0068(8)	0.0016(8)

I(1)	0.0215(1)	0.0197(1)	0.0271(1)	-0.0048(1)	0.0098(1)	-0.0027(1)

Table 4. Bond lengths [Å] for uvic1304_x.

atom-atom	distance	atom-atom	distance
P(1)-C(13)	1.7911(19)	P(1)-C(7)	1.7927(19)
P(1)-C(1)	1.795(2)	P(1)-C(19)	1.7979(19)
C(1)-C(2)	1.541(3)	C(2)-C(3)	1.516(3)
C(3)-C(4)	1.530(3)	C(4)-C(5)	1.484(4)
C(5)-C(6)	1.118(3)	C(7)-C(12)	1.389(3)
C(7)-C(8)	1.398(3)	C(8)-C(9)	1.382(3)
C(9)-C(10)	1.384(3)	C(10)-C(11)	1.380(3)
C(11)-C(12)	1.391(3)	C(13)-C(14)	1.396(3)
C(13)-C(18)	1.401(3)	C(14)-C(15)	1.389(3)
C(15)-C(16)	1.378(3)	C(16)-C(17)	1.388(3)
C(17)-C(18)	1.381(3)	C(19)-C(20)	1.396(3)
C(19)-C(24)	1.399(3)	C(20)-C(21)	1.387(3)
C(21)-C(22)	1.382(3)	C(22)-C(23)	1.388(3)
C(23)-C(24)	1.398(3)	C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900	C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900	C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900	C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900	C(6)-H(6)	0.9500
C(8)-H(8)	0.9500	C(9)-H(9)	0.9500
C(10)-H(10)	0.9500	C(11)-H(11)	0.9500
C(12)-H(12)	0.9500	C(14)-H(14)	0.9500
C(15)-H(15)	0.9500	C(16)-H(16)	0.9500
C(17)-H(17)	0.9500	C(18)-H(18)	0.9500
C(20)-H(20)	0.9500	C(21)-H(21)	0.9500
C(22)-H(22)	0.9500	C(23)-H(23)	0.9500

C(24)-H(24) 0.9500

Symmetry transformations used to generate equivalent atoms:

Table 5. Bond angles [°] for uvic1304_x.

atom-atom-atom	angle	atom-atom-atom	angle
C(13)-P(1)-C(7)	107.69(9)	C(13)-P(1)-C(1)	112.16(9)
C(7)-P(1)-C(1)	107.16(9)	C(13)-P(1)-C(19)	106.39(9)
C(7)-P(1)-C(19)	112.32(9)	C(1)-P(1)-C(19)	111.14(9)
C(2)-C(1)-P(1)	110.44(13)	C(3)-C(2)-C(1)	111.73(17)
C(2)-C(3)-C(4)	112.57(18)	C(5)-C(4)-C(3)	113.24(19)
C(6)-C(5)-C(4)	177.7(3)	C(12)-C(7)-C(8)	120.15(17)
C(12)-C(7)-P(1)	124.00(14)	C(8)-C(7)-P(1)	115.80(14)
C(9)-C(8)-C(7)	119.44(18)	C(8)-C(9)-C(10)	120.39(19)
C(11)-C(10)-C(9)	120.27(19)	C(10)-C(11)-C(12)	120.07(19)
C(7)-C(12)-C(11)	119.67(18)	C(14)-C(13)-C(18)	120.33(17)
C(14)-C(13)-P(1)	120.11(14)	C(18)-C(13)-P(1)	119.13(14)
C(15)-C(14)-C(13)	119.06(18)	C(16)-C(15)-C(14)	120.66(18)
C(15)-C(16)-C(17)	120.21(18)	C(18)-C(17)-C(16)	120.31(19)
C(17)-C(18)-C(13)	119.42(18)	C(20)-C(19)-C(24)	120.07(17)
C(20)-C(19)-P(1)	118.67(14)	C(24)-C(19)-P(1)	120.80(15)
C(21)-C(20)-C(19)	119.81(19)	C(22)-C(21)-C(20)	120.5(2)
C(21)-C(22)-C(23)	120.01(19)	C(22)-C(23)-C(24)	120.36(19)
C(23)-C(24)-C(19)	119.23(19)	C(2)-C(1)-H(1A)	109.6
P(1)-C(1)-H(1A)	109.6	C(2)-C(1)-H(1B)	109.6
P(1)-C(1)-H(1B)	109.6	H(1A)-C(1)-H(1B)	108.1
C(3)-C(2)-H(2A)	109.3	C(1)-C(2)-H(2A)	109.3
C(3)-C(2)-H(2B)	109.3	C(1)-C(2)-H(2B)	109.3
H(2A)-C(2)-H(2B)	107.9	C(2)-C(3)-H(3A)	109.1

C(4)-C(3)-H(3A)	109.1	C(2)-C(3)-H(3B)	109.1
C(4)-C(3)-H(3B)	109.1	H(3A)-C(3)-H(3B)	107.8
C(5)-C(4)-H(4A)	108.9	C(3)-C(4)-H(4A)	108.9
C(5)-C(4)-H(4B)	108.9	C(3)-C(4)-H(4B)	108.9
H(4A)-C(4)-H(4B)	107.7	C(5)-C(6)-H(6)	180.0
C(9)-C(8)-H(8)	120.3	C(7)-C(8)-H(8)	120.3
C(8)-C(9)-H(9)	119.8	C(10)-C(9)-H(9)	119.8
C(11)-C(10)-H(10)	119.9	C(9)-C(10)-H(10)	119.9
C(10)-C(11)-H(11)	120.0	C(12)-C(11)-H(11)	120.0
C(7)-C(12)-H(12)	120.2	C(11)-C(12)-H(12)	120.2
C(15)-C(14)-H(14)	120.5	C(13)-C(14)-H(14)	120.5
C(16)-C(15)-H(15)	119.7	C(14)-C(15)-H(15)	119.7
C(15)-C(16)-H(16)	119.9	C(17)-C(16)-H(16)	119.9
C(18)-C(17)-H(17)	119.8	C(16)-C(17)-H(17)	119.8
C(17)-C(18)-H(18)	120.3	C(13)-C(18)-H(18)	120.3
C(21)-C(20)-H(20)	120.1	C(19)-C(20)-H(20)	120.1
C(22)-C(21)-H(21)	119.7	C(20)-C(21)-H(21)	119.7
C(21)-C(22)-H(22)	120.0	C(23)-C(22)-H(22)	120.0
C(22)-C(23)-H(23)	119.8	C(24)-C(23)-H(23)	119.8
C(23)-C(24)-H(24)	120.4	C(19)-C(24)-H(24)	120.4

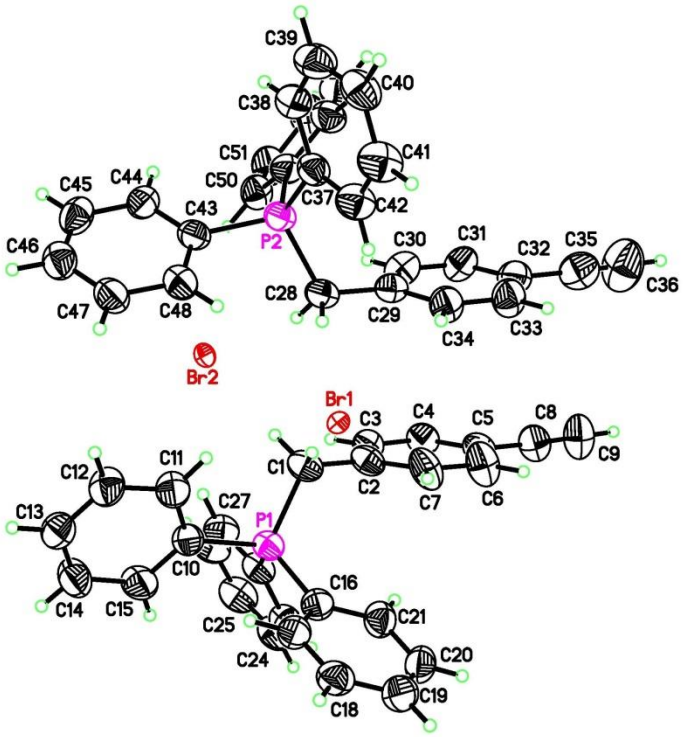
Symmetry transformations used to generate equivalent atoms:

Table 6. Torsion angles [°] for uvic1304_x.

atom-atom-atom-atom	angle	atom-atom-atom-atom	angle
C(13)-P(1)-C(1)-C(2)	-171.15(13)	C(7)-P(1)-C(1)-C(2)	-53.16(16)
C(19)-P(1)-C(1)-C(2)	69.90(16)	P(1)-C(1)-C(2)-C(3)	-178.70(15)
C(1)-C(2)-C(3)-C(4)	-174.04(18)	C(2)-C(3)-C(4)-C(5)	-59.7(3)
C(13)-P(1)-C(7)-C(12)	-129.77(17)	C(1)-P(1)-C(7)-C(12)	109.37(17)
C(19)-P(1)-C(7)-C(12)	-13.0(2)	C(13)-P(1)-C(7)-C(8)	52.73(17)
C(1)-P(1)-C(7)-C(8)	-68.13(17)	C(19)-P(1)-C(7)-C(8)	169.55(15)
C(12)-C(7)-C(8)-C(9)	1.1(3)	P(1)-C(7)-C(8)-C(9)	178.72(16)
C(7)-C(8)-C(9)-C(10)	-0.7(3)	C(8)-C(9)-C(10)-C(11)	-0.2(3)
C(9)-C(10)-C(11)-C(12)	0.6(3)	C(8)-C(7)-C(12)-C(11)	-0.7(3)
P(1)-C(7)-C(12)-C(11)	-178.12(16)	C(10)-C(11)-C(12)-C(7)	-0.1(3)
C(7)-P(1)-C(13)-C(14)	-156.87(15)	C(1)-P(1)-C(13)-C(14)	-39.20(18)
C(19)-P(1)-C(13)-C(14)	82.51(17)	C(7)-P(1)-C(13)-C(18)	30.58(18)
C(1)-P(1)-C(13)-C(18)	148.25(15)	C(19)-P(1)-C(13)-C(18)	-90.04(17)
C(18)-C(13)-C(14)-C(15)	-0.3(3)	P(1)-C(13)-C(14)-C(15)	-172.73(15)
C(13)-C(14)-C(15)-C(16)	0.0(3)	C(14)-C(15)-C(16)-C(17)	-0.2(3)
C(15)-C(16)-C(17)-C(18)	0.6(3)	C(16)-C(17)-C(18)-C(13)	-0.8(3)
C(14)-C(13)-C(18)-C(17)	0.7(3)	P(1)-C(13)-C(18)-C(17)	173.20(16)
C(13)-P(1)-C(19)-C(20)	72.36(17)	C(7)-P(1)-C(19)-C(20)	-45.23(18)
C(1)-P(1)-C(19)-C(20)	-165.27(15)	C(13)-P(1)-C(19)-C(24)	-99.80(16)
C(7)-P(1)-C(19)-C(24)	142.61(15)	C(1)-P(1)-C(19)-C(24)	22.56(18)
C(24)-C(19)-C(20)-C(21)	1.0(3)	P(1)-C(19)-C(20)-C(21)	-171.19(15)
C(19)-C(20)-C(21)-C(22)	-0.6(3)	C(20)-C(21)-C(22)-C(23)	-0.3(3)
C(21)-C(22)-C(23)-C(24)	0.7(3)	C(22)-C(23)-C(24)-C(19)	-0.3(3)
C(20)-C(19)-C(24)-C(23)	-0.6(3)	P(1)-C(19)-C(24)-C(23)	171.46(15)

Symmetry transformations used to generate equivalent atoms:

Table S5. Crystal data and structure refinement for (4-ethynylbenzyl)triphenylphosphonium hexafluorophosphate(V).



Identification code	uvic1217	
Empirical formula	$C_{27}H_{22}BrP$	
Formula weight	457.33	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.8176(15) Å	α = 98.278(3)°
	b = 12.4498(18) Å	β = 94.561(3)°
	c = 18.455(3) Å	γ = 107.751(3)°

Volume	2322.3(6) $Å^3$
Z	4
Density (calculated)	1.308 $g.cm^{-3}$
Absorption coefficient (μ)	1.849 mm^{-1}
F(000)	936
Crystal color, habit	light brown, tablet
Crystal size	0.22 × 0.15 × 0.08 mm^3
θ range for data collection	1.12 to 26.41°
Index ranges	$-13 \leq h \leq 13$, $-15 \leq k \leq 15$, $-23 \leq l \leq 23$
Reflections collected	47622
Independent reflections	9517 [R_{int} = 0.0384]
Completeness to θ = 26.41°	99.7 %
Absorption correction	Numerical
Max. and min. transmission	0.9390 and 0.7946
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9517 / 0 / 523
Goodness-of-fit on F^2	1.066
Final R indices [I>2σ(I)]	R_1 = 0.0666, wR_2 = 0.2057
R indices (all data)	R_1 = 0.0792, wR_2 = 0.2208
Largest diff. peak and hole	2.125 and -1.731 $e^-.Å^{-3}$

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for uvic1217. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Br(1)	0.77064(4)	-0.00819(4)	0.13317(2)	0.016(1)
Br(2)	0.54519(5)	0.42038(4)	0.26878(3)	0.027(1)
P(1)	0.88338(17)	0.39375(14)	0.12470(10)	0.039(1)
C(1)	0.8298(7)	0.3242(6)	0.2018(4)	0.046(2)
C(2)	0.9266(7)	0.3632(6)	0.2713(4)	0.044(2)
C(3)	0.9253(7)	0.4538(6)	0.3238(4)	0.045(2)
C(4)	1.0120(7)	0.4873(6)	0.3887(4)	0.047(2)
C(5)	1.1034(8)	0.4337(6)	0.4019(4)	0.049(2)
C(6)	1.1048(10)	0.3411(8)	0.3492(5)	0.064(2)
C(7)	1.0144(9)	0.3062(7)	0.2851(4)	0.058(2)
C(8)	1.1943(8)	0.4687(7)	0.4686(4)	0.056(2)
C(9)	1.2666(10)	0.4967(8)	0.5252(5)	0.068(2)
C(10)	0.7475(7)	0.3482(6)	0.0529(4)	0.042(2)
C(11)	0.6497(7)	0.2417(6)	0.0490(4)	0.051(2)
C(12)	0.5472(8)	0.2075(6)	-0.0086(5)	0.055(2)
C(13)	0.5379(8)	0.2765(7)	-0.0588(5)	0.056(2)
C(14)	0.6313(9)	0.3817(8)	-0.0538(5)	0.067(2)
C(15)	0.7377(8)	0.4165(7)	0.0011(5)	0.058(2)
C(16)	1.0192(7)	0.3546(6)	0.0933(4)	0.045(2)
C(17)	1.0006(7)	0.2812(6)	0.0254(4)	0.045(2)
C(18)	1.1030(8)	0.2457(7)	0.0031(5)	0.054(2)
C(19)	1.2229(9)	0.2812(8)	0.0484(5)	0.060(2)
C(20)	1.2411(8)	0.3524(7)	0.1148(5)	0.058(2)
C(21)	1.1389(7)	0.3889(7)	0.1391(5)	0.052(2)
C(22)	0.9239(7)	0.5465(6)	0.1508(4)	0.043(2)
C(23)	1.0471(8)	0.6234(6)	0.1488(4)	0.050(2)

C(24)	1.0706(9)	0.7392(7)	0.1688(5)	0.059(2)
C(25)	0.9685(10)	0.7797(7)	0.1902(5)	0.062(2)
C(26)	0.8474(9)	0.7047(7)	0.1900(5)	0.059(2)
C(27)	0.8242(8)	0.5876(6)	0.1720(4)	0.052(2)
P(2)	0.44593(17)	0.03327(15)	0.30060(10)	0.039(1)
C(28)	0.6126(7)	0.1159(6)	0.2943(4)	0.044(2)
C(29)	0.7112(7)	0.1331(6)	0.3613(4)	0.044(2)
C(30)	0.7149(8)	0.2091(6)	0.4242(5)	0.053(2)
C(31)	0.8016(7)	0.2247(7)	0.4842(5)	0.053(2)
C(32)	0.8917(8)	0.1677(8)	0.4859(4)	0.056(2)
C(33)	0.8924(8)	0.0913(8)	0.4231(4)	0.057(2)
C(34)	0.8039(8)	0.0746(7)	0.3605(4)	0.052(2)
C(35)	0.9886(10)	0.1879(8)	0.5555(6)	0.067(2)
C(36)	1.0546(13)	0.2046(12)	0.6059(7)	0.101(4)
C(37)	0.4248(7)	-0.1151(6)	0.3026(4)	0.043(2)
C(38)	0.3085(8)	-0.1832(7)	0.3205(4)	0.052(2)
C(39)	0.2852(9)	-0.2981(7)	0.3183(5)	0.059(2)
C(40)	0.3786(9)	-0.3476(7)	0.2983(5)	0.056(2)
C(41)	0.4940(9)	-0.2814(7)	0.2781(5)	0.061(2)
C(42)	0.5186(8)	-0.1644(7)	0.2794(4)	0.054(2)
C(43)	0.3452(7)	0.0377(6)	0.2196(4)	0.043(2)
C(44)	0.2301(7)	0.0638(6)	0.2233(4)	0.045(2)
C(45)	0.1523(8)	0.0571(7)	0.1576(5)	0.054(2)
C(46)	0.1874(8)	0.0247(6)	0.0907(5)	0.053(2)
C(47)	0.3040(8)	-0.0030(7)	0.0859(4)	0.052(2)
C(48)	0.3841(8)	0.0042(7)	0.1509(4)	0.051(2)
C(49)	0.3985(7)	0.0977(6)	0.3832(4)	0.046(2)
C(50)	0.3903(7)	0.2068(7)	0.3855(4)	0.050(2)
C(51)	0.3763(9)	0.2689(8)	0.4519(5)	0.062(2)
C(52)	0.3646(10)	0.2167(10)	0.5146(5)	0.074(3)
C(53)	0.3733(9)	0.1092(9)	0.5122(5)	0.069(2)

C(54)	0.3895(8)	0.0473(7)	0.4457(4)	0.053(2)
H(1A)	0.7474	0.3378	0.2133	0.055
H(1B)	0.8099	0.2406	0.1864	0.055
H(3)	0.8646	0.4934	0.3154	0.054
H(4)	1.0082	0.5485	0.4248	0.056
H(6)	1.1667	0.3024	0.3570	0.077
H(7)	1.0135	0.2417	0.2503	0.069
H(9)	1.3242	0.5190	0.5703	0.081
H(11)	0.6537	0.1946	0.0847	0.061
H(12)	0.4822	0.1347	-0.0132	0.066
H(13)	0.4665	0.2514	-0.0974	0.067
H(14)	0.6230	0.4304	-0.0878	0.081
H(15)	0.8044	0.4877	0.0032	0.070
H(17)	0.9185	0.2561	-0.0049	0.054
H(18)	1.0917	0.1971	-0.0433	0.065
H(19)	1.2924	0.2557	0.0330	0.072
H(20)	1.3237	0.3772	0.1446	0.070
H(21)	1.1506	0.4363	0.1860	0.062
H(23)	1.1153	0.5956	0.1336	0.060
H(24)	1.1552	0.7916	0.1680	0.071
H(25)	0.9844	0.8596	0.2049	0.075
H(26)	0.7778	0.7327	0.2024	0.071
H(27)	0.7401	0.5355	0.1741	0.063
H(28A)	0.6417	0.0777	0.2512	0.053
H(28B)	0.6135	0.1923	0.2845	0.053
H(30)	0.6550	0.2513	0.4252	0.063
H(31)	0.8004	0.2769	0.5269	0.064
H(33)	0.9536	0.0504	0.4230	0.068
H(34)	0.8059	0.0238	0.3173	0.062
H(36)	1.1127	0.2193	0.6502	0.122
H(38)	0.2438	-0.1499	0.3344	0.062

H(39)	0.2046	-0.3440	0.3305	0.071
H(40)	0.3636	-0.4268	0.2986	0.068
H(41)	0.5571	-0.3160	0.2630	0.073
H(42)	0.5974	-0.1190	0.2650	0.064
H(44)	0.2044	0.0859	0.2697	0.054
H(45)	0.0735	0.0754	0.1596	0.065
H(46)	0.1328	0.0207	0.0468	0.064
H(47)	0.3277	-0.0263	0.0392	0.063
H(48)	0.4636	-0.0131	0.1489	0.061
H(50)	0.3942	0.2395	0.3419	0.060
H(51)	0.3748	0.3453	0.4545	0.074
H(52)	0.3505	0.2568	0.5594	0.088
H(53)	0.3683	0.0761	0.5556	0.082
H(54)	0.3942	-0.0280	0.4436	0.064

Table 3. Anisotropic displacement parameters ($Å^2$) for uvic1217.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br(1)	0.0158(2)	0.0150(2)	0.0170(2)	-0.0009(2)	0.0019(2)	0.0043(2)
Br(2)	0.0285(3)	0.0280(3)	0.0295(3)	0.0119(2)	0.0028(2)	0.0120(2)
P(1)	0.0417(9)	0.0315(8)	0.0380(9)	0.0056(7)	0.0037(7)	0.0058(7)
C(1)	0.057(4)	0.031(3)	0.048(4)	0.010(3)	0.010(3)	0.010(3)
C(2)	0.058(4)	0.032(3)	0.039(3)	0.008(3)	0.007(3)	0.010(3)
C(3)	0.050(4)	0.042(4)	0.045(4)	0.008(3)	0.007(3)	0.017(3)
C(4)	0.056(4)	0.044(4)	0.040(4)	0.002(3)	0.009(3)	0.019(3)
C(5)	0.066(5)	0.046(4)	0.041(4)	0.009(3)	0.011(3)	0.023(4)
C(6)	0.088(6)	0.062(5)	0.050(4)	0.000(4)	-0.004(4)	0.042(5)
C(7)	0.088(6)	0.051(4)	0.041(4)	0.004(3)	-0.001(4)	0.037(4)
C(8)	0.066(5)	0.058(5)	0.047(4)	0.004(4)	0.005(4)	0.030(4)
C(9)	0.080(6)	0.072(6)	0.055(5)	-0.008(4)	-0.010(4)	0.044(5)
C(10)	0.042(4)	0.042(4)	0.041(3)	0.006(3)	0.005(3)	0.013(3)
C(11)	0.051(4)	0.039(4)	0.058(4)	0.012(3)	-0.002(3)	0.006(3)
C(12)	0.049(4)	0.041(4)	0.062(5)	0.005(3)	-0.005(4)	0.003(3)
C(13)	0.045(4)	0.055(5)	0.057(5)	0.010(4)	-0.002(3)	0.004(3)
C(14)	0.064(5)	0.063(5)	0.062(5)	0.028(4)	-0.011(4)	0.000(4)
C(15)	0.055(5)	0.047(4)	0.058(5)	0.017(4)	0.000(4)	-0.006(3)
C(16)	0.041(4)	0.040(4)	0.050(4)	0.013(3)	0.003(3)	0.004(3)
C(17)	0.045(4)	0.043(4)	0.049(4)	0.011(3)	0.006(3)	0.013(3)
C(18)	0.061(5)	0.053(4)	0.056(5)	0.019(4)	0.016(4)	0.023(4)
C(19)	0.057(5)	0.063(5)	0.071(6)	0.027(4)	0.016(4)	0.027(4)
C(20)	0.042(4)	0.060(5)	0.077(6)	0.030(4)	0.002(4)	0.016(4)
C(21)	0.048(4)	0.050(4)	0.054(4)	0.010(3)	-0.002(3)	0.012(3)
C(22)	0.056(4)	0.032(3)	0.037(3)	0.005(3)	0.004(3)	0.009(3)

C(23)	0.054(4)	0.044(4)	0.043(4)	0.008(3)	0.000(3)	0.005(3)
C(24)	0.069(5)	0.039(4)	0.057(5)	0.013(3)	-0.001(4)	0.001(4)
C(25)	0.086(6)	0.039(4)	0.060(5)	0.008(4)	0.011(4)	0.016(4)
C(26)	0.078(6)	0.040(4)	0.061(5)	0.012(4)	0.016(4)	0.018(4)
C(27)	0.058(4)	0.041(4)	0.058(4)	0.011(3)	0.012(4)	0.013(3)
P(2)	0.0425(9)	0.0395(9)	0.0400(9)	0.0115(7)	0.0103(7)	0.0153(7)
C(28)	0.049(4)	0.043(4)	0.044(4)	0.014(3)	0.014(3)	0.015(3)
C(29)	0.043(4)	0.042(4)	0.046(4)	0.012(3)	0.010(3)	0.010(3)
C(30)	0.048(4)	0.044(4)	0.062(5)	-0.001(3)	0.007(4)	0.013(3)
C(31)	0.043(4)	0.060(5)	0.052(4)	-0.001(4)	0.004(3)	0.015(3)
C(32)	0.048(4)	0.065(5)	0.049(4)	0.011(4)	0.002(3)	0.009(4)
C(33)	0.061(5)	0.070(5)	0.051(4)	0.009(4)	0.010(4)	0.036(4)
C(34)	0.056(4)	0.059(5)	0.047(4)	0.008(3)	0.009(3)	0.027(4)
C(35)	0.065(5)	0.068(6)	0.065(6)	0.003(4)	0.012(5)	0.019(4)
C(36)	0.093(8)	0.139(12)	0.064(7)	-0.014(7)	-0.010(6)	0.047(8)
C(37)	0.047(4)	0.040(3)	0.045(4)	0.013(3)	0.006(3)	0.015(3)
C(38)	0.051(4)	0.049(4)	0.056(4)	0.017(3)	0.008(3)	0.014(3)
C(39)	0.065(5)	0.045(4)	0.061(5)	0.015(4)	0.010(4)	0.007(4)
C(40)	0.074(5)	0.037(4)	0.059(5)	0.014(3)	0.006(4)	0.019(4)
C(41)	0.075(6)	0.046(4)	0.069(5)	0.013(4)	0.022(4)	0.027(4)
C(42)	0.062(5)	0.048(4)	0.056(4)	0.012(3)	0.016(4)	0.021(4)
C(43)	0.046(4)	0.043(4)	0.041(4)	0.013(3)	0.009(3)	0.012(3)
C(44)	0.041(4)	0.043(4)	0.051(4)	0.009(3)	0.005(3)	0.013(3)
C(45)	0.043(4)	0.046(4)	0.075(6)	0.012(4)	0.002(4)	0.016(3)
C(46)	0.054(4)	0.045(4)	0.055(4)	0.009(3)	-0.004(4)	0.010(3)
C(47)	0.058(4)	0.054(4)	0.042(4)	0.014(3)	0.004(3)	0.013(4)
C(48)	0.053(4)	0.059(5)	0.044(4)	0.015(3)	0.007(3)	0.020(4)
C(49)	0.044(4)	0.053(4)	0.042(4)	0.011(3)	0.011(3)	0.015(3)
C(50)	0.053(4)	0.053(4)	0.049(4)	0.008(3)	0.008(3)	0.026(3)
C(51)	0.071(5)	0.068(5)	0.055(5)	0.004(4)	0.009(4)	0.036(5)
C(52)	0.086(7)	0.105(8)	0.047(5)	0.006(5)	0.021(4)	0.056(6)

C(53)	0.071(6)	0.090(7)	0.052(5)	0.020(5)	0.020(4)	0.031(5)
C(54)	0.058(5)	0.061(5)	0.046(4)	0.016(3)	0.016(3)	0.022(4)

Table 4. Bond lengths [Å] for uvic1217.

atom-atom	distance	atom-atom	distance
P(1)-C(10)	1.790(7)	P(1)-C(16)	1.795(8)
P(1)-C(22)	1.799(7)	P(1)-C(1)	1.814(7)
C(1)-C(2)	1.508(10)	C(2)-C(7)	1.377(11)
C(2)-C(3)	1.381(10)	C(3)-C(4)	1.389(10)
C(4)-C(5)	1.375(10)	C(5)-C(6)	1.401(11)
C(5)-C(8)	1.436(11)	C(6)-C(7)	1.398(11)
C(8)-C(9)	1.194(12)	C(10)-C(15)	1.386(10)
C(10)-C(11)	1.410(10)	C(11)-C(12)	1.391(10)
C(12)-C(13)	1.368(11)	C(13)-C(14)	1.375(11)
C(14)-C(15)	1.387(11)	C(16)-C(21)	1.400(10)
C(16)-C(17)	1.401(10)	C(17)-C(18)	1.382(10)
C(18)-C(19)	1.396(12)	C(19)-C(20)	1.366(13)
C(20)-C(21)	1.399(11)	C(22)-C(27)	1.387(11)
C(22)-C(23)	1.390(10)	C(23)-C(24)	1.374(11)
C(24)-C(25)	1.409(13)	C(25)-C(26)	1.357(12)
C(26)-C(27)	1.388(10)	P(2)-C(43)	1.796(7)
P(2)-C(37)	1.797(7)	P(2)-C(49)	1.803(7)
P(2)-C(28)	1.805(7)	C(28)-C(29)	1.513(10)
C(29)-C(30)	1.378(10)	C(29)-C(34)	1.407(10)
C(30)-C(31)	1.344(11)	C(31)-C(32)	1.371(11)
C(32)-C(33)	1.391(11)	C(32)-C(35)	1.531(13)
C(33)-C(34)	1.389(11)	C(35)-C(36)	1.078(14)
C(37)-C(38)	1.381(10)	C(37)-C(42)	1.401(10)
C(38)-C(39)	1.368(11)	C(39)-C(40)	1.382(12)
C(40)-C(41)	1.383(12)	C(41)-C(42)	1.395(11)
C(43)-C(44)	1.384(10)	C(43)-C(48)	1.414(10)
C(44)-C(45)	1.396(11)	C(45)-C(46)	1.363(12)

C(46)-C(47)	1.411(11)	C(47)-C(48)	1.397(10)
C(49)-C(50)	1.383(10)	C(49)-C(54)	1.386(10)
C(50)-C(51)	1.397(11)	C(51)-C(52)	1.403(13)
C(52)-C(53)	1.365(14)	C(53)-C(54)	1.406(12)
C(1)-H(1A)	0.9900	C(1)-H(1B)	0.9900
C(3)-H(3)	0.9500	C(4)-H(4)	0.9500
C(6)-H(6)	0.9500	C(7)-H(7)	0.9500
C(9)-H(9)	0.9500	C(11)-H(11)	0.9500
C(12)-H(12)	0.9500	C(13)-H(13)	0.9500
C(14)-H(14)	0.9500	C(15)-H(15)	0.9500
C(17)-H(17)	0.9500	C(18)-H(18)	0.9500
C(19)-H(19)	0.9500	C(20)-H(20)	0.9500
C(21)-H(21)	0.9500	C(23)-H(23)	0.9500
C(24)-H(24)	0.9500	C(25)-H(25)	0.9500
C(26)-H(26)	0.9500	C(27)-H(27)	0.9500
C(28)-H(28A)	0.9900	C(28)-H(28B)	0.9900
C(30)-H(30)	0.9500	C(31)-H(31)	0.9500
C(33)-H(33)	0.9500	C(34)-H(34)	0.9500
C(36)-H(36)	0.9500	C(38)-H(38)	0.9500
C(39)-H(39)	0.9500	C(40)-H(40)	0.9500
C(41)-H(41)	0.9500	C(42)-H(42)	0.9500
C(44)-H(44)	0.9500	C(45)-H(45)	0.9500
C(46)-H(46)	0.9500	C(47)-H(47)	0.9500
C(48)-H(48)	0.9500	C(50)-H(50)	0.9500
C(51)-H(51)	0.9500	C(52)-H(52)	0.9500
C(53)-H(53)	0.9500	C(54)-H(54)	0.9500

Symmetry transformations used to generate equivalent atoms:

Table 5. Bond angles [°] for uvic1217.

atom-atom-atom	angle	atom-atom-atom	angle
C(10)-P(1)-C(16)	110.6(3)	C(10)-P(1)-C(22)	106.8(3)
C(16)-P(1)-C(22)	111.7(3)	C(10)-P(1)-C(1)	107.5(3)
C(16)-P(1)-C(1)	110.1(3)	C(22)-P(1)-C(1)	110.1(3)
C(2)-C(1)-P(1)	115.1(5)	C(7)-C(2)-C(3)	118.6(7)
C(7)-C(2)-C(1)	120.6(6)	C(3)-C(2)-C(1)	120.7(7)
C(2)-C(3)-C(4)	120.6(7)	C(5)-C(4)-C(3)	121.3(7)
C(4)-C(5)-C(6)	118.6(7)	C(4)-C(5)-C(8)	121.6(7)
C(6)-C(5)-C(8)	119.8(7)	C(7)-C(6)-C(5)	119.4(8)
C(2)-C(7)-C(6)	121.4(7)	C(9)-C(8)-C(5)	178.0(10)
C(15)-C(10)-C(11)	119.8(7)	C(15)-C(10)-P(1)	120.6(5)
C(11)-C(10)-P(1)	119.6(5)	C(12)-C(11)-C(10)	118.1(7)
C(13)-C(12)-C(11)	121.4(7)	C(12)-C(13)-C(14)	120.4(7)
C(13)-C(14)-C(15)	119.7(8)	C(10)-C(15)-C(14)	120.5(7)
C(21)-C(16)-C(17)	120.4(7)	C(21)-C(16)-P(1)	120.2(6)
C(17)-C(16)-P(1)	119.2(5)	C(18)-C(17)-C(16)	119.3(7)
C(17)-C(18)-C(19)	120.1(8)	C(20)-C(19)-C(18)	120.6(8)
C(19)-C(20)-C(21)	120.5(8)	C(20)-C(21)-C(16)	119.0(8)
C(27)-C(22)-C(23)	119.6(7)	C(27)-C(22)-P(1)	116.9(5)
C(23)-C(22)-P(1)	123.5(6)	C(24)-C(23)-C(22)	120.3(8)
C(23)-C(24)-C(25)	119.5(8)	C(26)-C(25)-C(24)	120.1(8)
C(25)-C(26)-C(27)	120.6(9)	C(22)-C(27)-C(26)	119.9(7)
C(43)-P(2)-C(37)	106.9(3)	C(43)-P(2)-C(49)	111.1(3)
C(37)-P(2)-C(49)	110.0(3)	C(43)-P(2)-C(28)	107.9(3)
C(37)-P(2)-C(28)	113.1(3)	C(49)-P(2)-C(28)	107.7(3)
C(29)-C(28)-P(2)	116.1(5)	C(30)-C(29)-C(34)	118.2(7)
C(30)-C(29)-C(28)	120.6(7)	C(34)-C(29)-C(28)	121.1(7)
C(31)-C(30)-C(29)	121.2(8)	C(30)-C(31)-C(32)	122.2(8)

C(31)-C(32)-C(33)	118.4(7)	C(31)-C(32)-C(35)	120.4(8)
C(33)-C(32)-C(35)	121.2(8)	C(34)-C(33)-C(32)	120.2(8)
C(33)-C(34)-C(29)	119.8(7)	C(36)-C(35)-C(32)	177.4(12)
C(38)-C(37)-C(42)	119.9(7)	C(38)-C(37)-P(2)	118.9(6)
C(42)-C(37)-P(2)	120.9(6)	C(39)-C(38)-C(37)	120.8(8)
C(38)-C(39)-C(40)	120.2(8)	C(39)-C(40)-C(41)	119.8(7)
C(40)-C(41)-C(42)	120.6(8)	C(41)-C(42)-C(37)	118.6(7)
C(44)-C(43)-C(48)	121.1(7)	C(44)-C(43)-P(2)	122.3(5)
C(48)-C(43)-P(2)	116.4(6)	C(43)-C(44)-C(45)	118.8(7)
C(46)-C(45)-C(44)	121.3(7)	C(45)-C(46)-C(47)	120.7(7)
C(48)-C(47)-C(46)	119.1(7)	C(47)-C(48)-C(43)	119.0(7)
C(50)-C(49)-C(54)	120.9(7)	C(50)-C(49)-P(2)	117.3(5)
C(54)-C(49)-P(2)	121.2(6)	C(49)-C(50)-C(51)	119.9(8)
C(50)-C(51)-C(52)	118.9(8)	C(53)-C(52)-C(51)	120.9(8)
C(52)-C(53)-C(54)	120.2(8)	C(49)-C(54)-C(53)	119.1(8)
C(2)-C(1)-H(1A)	108.5	P(1)-C(1)-H(1A)	108.5
C(2)-C(1)-H(1B)	108.5	P(1)-C(1)-H(1B)	108.5
H(1A)-C(1)-H(1B)	107.5	C(2)-C(3)-H(3)	119.7
C(4)-C(3)-H(3)	119.7	C(5)-C(4)-H(4)	119.4
C(3)-C(4)-H(4)	119.4	C(7)-C(6)-H(6)	120.3
C(5)-C(6)-H(6)	120.3	C(2)-C(7)-H(7)	119.3
C(6)-C(7)-H(7)	119.3	C(8)-C(9)-H(9)	180.0
C(12)-C(11)-H(11)	120.9	C(10)-C(11)-H(11)	120.9
C(13)-C(12)-H(12)	119.3	C(11)-C(12)-H(12)	119.3
C(12)-C(13)-H(13)	119.8	C(14)-C(13)-H(13)	119.8
C(13)-C(14)-H(14)	120.2	C(15)-C(14)-H(14)	120.2
C(10)-C(15)-H(15)	119.8	C(14)-C(15)-H(15)	119.8
C(18)-C(17)-H(17)	120.3	C(16)-C(17)-H(17)	120.3
C(17)-C(18)-H(18)	119.9	C(19)-C(18)-H(18)	119.9
C(20)-C(19)-H(19)	119.7	C(18)-C(19)-H(19)	119.7
C(19)-C(20)-H(20)	119.8	C(21)-C(20)-H(20)	119.8

C(20)-C(21)-H(21)	120.5	C(16)-C(21)-H(21)	120.5
C(24)-C(23)-H(23)	119.8	C(22)-C(23)-H(23)	119.8
C(23)-C(24)-H(24)	120.3	C(25)-C(24)-H(24)	120.3
C(26)-C(25)-H(25)	120.0	C(24)-C(25)-H(25)	120.0
C(25)-C(26)-H(26)	119.7	C(27)-C(26)-H(26)	119.7
C(22)-C(27)-H(27)	120.0	C(26)-C(27)-H(27)	120.0
C(29)-C(28)-H(28A)	108.3	P(2)-C(28)-H(28A)	108.3
C(29)-C(28)-H(28B)	108.3	P(2)-C(28)-H(28B)	108.3
H(28A)-C(28)-H(28B)	107.4	C(31)-C(30)-H(30)	119.4
C(29)-C(30)-H(30)	119.4	C(30)-C(31)-H(31)	118.9
C(32)-C(31)-H(31)	118.9	C(34)-C(33)-H(33)	119.9
C(32)-C(33)-H(33)	119.9	C(33)-C(34)-H(34)	120.1
C(29)-C(34)-H(34)	120.1	C(35)-C(36)-H(36)	180.0
C(39)-C(38)-H(38)	119.6	C(37)-C(38)-H(38)	119.6
C(38)-C(39)-H(39)	119.9	C(40)-C(39)-H(39)	119.9
C(39)-C(40)-H(40)	120.1	C(41)-C(40)-H(40)	120.1
C(40)-C(41)-H(41)	119.7	C(42)-C(41)-H(41)	119.7
C(41)-C(42)-H(42)	120.7	C(37)-C(42)-H(42)	120.7
C(43)-C(44)-H(44)	120.6	C(45)-C(44)-H(44)	120.6
C(46)-C(45)-H(45)	119.4	C(44)-C(45)-H(45)	119.4
C(45)-C(46)-H(46)	119.7	C(47)-C(46)-H(46)	119.7
C(48)-C(47)-H(47)	120.4	C(46)-C(47)-H(47)	120.4
C(47)-C(48)-H(48)	120.5	C(43)-C(48)-H(48)	120.5
C(49)-C(50)-H(50)	120.0	C(51)-C(50)-H(50)	120.0
C(50)-C(51)-H(51)	120.5	C(52)-C(51)-H(51)	120.5
C(53)-C(52)-H(52)	119.6	C(51)-C(52)-H(52)	119.6
C(52)-C(53)-H(53)	119.9	C(54)-C(53)-H(53)	119.9
C(49)-C(54)-H(54)	120.4	C(53)-C(54)-H(54)	120.4

Symmetry transformations used to generate equivalent atoms:

Table 6. Torsion angles [°] for uvic1217.

atom-atom-atom-atom	angle	atom-atom-atom-atom	angle
C(10)-P(1)-C(1)-C(2)	-173.0(5)	C(16)-P(1)-C(1)-C(2)	66.4(6)
C(22)-P(1)-C(1)-C(2)	-57.1(6)	P(1)-C(1)-C(2)-C(7)	-92.8(8)
P(1)-C(1)-C(2)-C(3)	90.0(8)	C(7)-C(2)-C(3)-C(4)	0.8(11)
C(1)-C(2)-C(3)-C(4)	178.1(6)	C(2)-C(3)-C(4)-C(5)	1.6(11)
C(3)-C(4)-C(5)-C(6)	-2.1(12)	C(3)-C(4)-C(5)-C(8)	179.3(7)
C(4)-C(5)-C(6)-C(7)	0.2(13)	C(8)-C(5)-C(6)-C(7)	178.8(8)
C(3)-C(2)-C(7)-C(6)	-2.7(12)	C(1)-C(2)-C(7)-C(6)	-180.0(8)
C(5)-C(6)-C(7)-C(2)	2.2(14)	C(4)-C(5)-C(8)-C(9)	66(25)
C(6)-C(5)-C(8)-C(9)	-113(25)	C(16)-P(1)-C(10)-C(15)	-85.9(7)
C(22)-P(1)-C(10)-C(15)	35.8(7)	C(1)-P(1)-C(10)-C(15)	153.9(7)
C(16)-P(1)-C(10)-C(11)	94.1(6)	C(22)-P(1)-C(10)-C(11)	-144.2(6)
C(1)-P(1)-C(10)-C(11)	-26.1(7)	C(15)-C(10)-C(11)-C(12)	1.6(12)
P(1)-C(10)-C(11)-C(12)	-178.4(6)	C(10)-C(11)-C(12)-C(13)	-2.4(13)
C(11)-C(12)-C(13)-C(14)	0.6(14)	C(12)-C(13)-C(14)-C(15)	2.1(15)
C(11)-C(10)-C(15)-C(14)	1.0(13)	P(1)-C(10)-C(15)-C(14)	-179.0(7)
C(13)-C(14)-C(15)-C(10)	-2.9(15)	C(10)-P(1)-C(16)-C(21)	175.6(6)
C(22)-P(1)-C(16)-C(21)	56.8(7)	C(1)-P(1)-C(16)-C(21)	-65.8(7)
C(10)-P(1)-C(16)-C(17)	-9.9(7)	C(22)-P(1)-C(16)-C(17)	-128.7(6)
C(1)-P(1)-C(16)-C(17)	108.7(6)	C(21)-C(16)-C(17)-C(18)	-1.9(11)
P(1)-C(16)-C(17)-C(18)	-176.4(5)	C(16)-C(17)-C(18)-C(19)	1.1(11)
C(17)-C(18)-C(19)-C(20)	-0.8(12)	C(18)-C(19)-C(20)-C(21)	1.3(12)
C(19)-C(20)-C(21)-C(16)	-2.1(12)	C(17)-C(16)-C(21)-C(20)	2.4(11)
P(1)-C(16)-C(21)-C(20)	176.8(6)	C(10)-P(1)-C(22)-C(27)	55.3(6)
C(16)-P(1)-C(22)-C(27)	176.4(6)	C(1)-P(1)-C(22)-C(27)	-61.1(7)
C(10)-P(1)-C(22)-C(23)	-122.9(6)	C(16)-P(1)-C(22)-C(23)	-1.9(7)
C(1)-P(1)-C(22)-C(23)	120.7(6)	C(27)-C(22)-C(23)-C(24)	1.0(11)
P(1)-C(22)-C(23)-C(24)	179.2(6)	C(22)-C(23)-C(24)-C(25)	-0.9(12)

C(23)-C(24)-C(25)-C(26)	-1.1(13)	C(24)-C(25)-C(26)-C(27)	2.9(13)
C(23)-C(22)-C(27)-C(26)	0.8(11)	P(1)-C(22)-C(27)-C(26)	-177.5(6)
C(25)-C(26)-C(27)-C(22)	-2.8(13)	C(43)-P(2)-C(28)-C(29)	173.9(5)
C(37)-P(2)-C(28)-C(29)	-68.0(6)	C(49)-P(2)-C(28)-C(29)	53.8(6)
P(2)-C(28)-C(29)-C(30)	-74.9(8)	P(2)-C(28)-C(29)-C(34)	107.0(7)
C(34)-C(29)-C(30)-C(31)	-2.1(11)	C(28)-C(29)-C(30)-C(31)	179.7(7)
C(29)-C(30)-C(31)-C(32)	1.0(13)	C(30)-C(31)-C(32)-C(33)	-0.1(13)
C(30)-C(31)-C(32)-C(35)	-179.9(8)	C(31)-C(32)-C(33)-C(34)	0.4(13)
C(35)-C(32)-C(33)-C(34)	-179.8(8)	C(32)-C(33)-C(34)-C(29)	-1.6(13)
C(30)-C(29)-C(34)-C(33)	2.4(11)	C(28)-C(29)-C(34)-C(33)	-179.4(7)
C(31)-C(32)-C(35)-C(36)	5(30)	C(33)-C(32)-C(35)-C(36)	-175(29)
C(43)-P(2)-C(37)-C(38)	-72.8(7)	C(49)-P(2)-C(37)-C(38)	48.0(7)
C(28)-P(2)-C(37)-C(38)	168.6(6)	C(43)-P(2)-C(37)-C(42)	100.9(7)
C(49)-P(2)-C(37)-C(42)	-138.3(6)	C(28)-P(2)-C(37)-C(42)	-17.7(7)
C(42)-C(37)-C(38)-C(39)	2.3(12)	P(2)-C(37)-C(38)-C(39)	176.0(6)
C(37)-C(38)-C(39)-C(40)	0.2(13)	C(38)-C(39)-C(40)-C(41)	-2.2(13)
C(39)-C(40)-C(41)-C(42)	1.7(13)	C(40)-C(41)-C(42)-C(37)	0.7(13)
C(38)-C(37)-C(42)-C(41)	-2.7(12)	P(2)-C(37)-C(42)-C(41)	-176.4(6)
C(37)-P(2)-C(43)-C(44)	106.8(6)	C(49)-P(2)-C(43)-C(44)	-13.3(7)
C(28)-P(2)-C(43)-C(44)	-131.2(6)	C(37)-P(2)-C(43)-C(48)	-68.3(6)
C(49)-P(2)-C(43)-C(48)	171.6(6)	C(28)-P(2)-C(43)-C(48)	53.7(6)
C(48)-C(43)-C(44)-C(45)	-0.3(11)	P(2)-C(43)-C(44)-C(45)	-175.3(6)
C(43)-C(44)-C(45)-C(46)	0.5(11)	C(44)-C(45)-C(46)-C(47)	-0.1(12)
C(45)-C(46)-C(47)-C(48)	-0.6(12)	C(46)-C(47)-C(48)-C(43)	0.8(11)
C(44)-C(43)-C(48)-C(47)	-0.4(11)	P(2)-C(43)-C(48)-C(47)	174.9(6)
C(43)-P(2)-C(49)-C(50)	-52.4(7)	C(37)-P(2)-C(49)-C(50)	-170.6(6)
C(28)-P(2)-C(49)-C(50)	65.6(7)	C(43)-P(2)-C(49)-C(54)	136.8(6)
C(37)-P(2)-C(49)-C(54)	18.6(8)	C(28)-P(2)-C(49)-C(54)	-105.1(7)
C(54)-C(49)-C(50)-C(51)	1.8(12)	P(2)-C(49)-C(50)-C(51)	-169.0(6)
C(49)-C(50)-C(51)-C(52)	-3.0(13)	C(50)-C(51)-C(52)-C(53)	3.3(15)
C(51)-C(52)-C(53)-C(54)	-2.3(15)	C(50)-C(49)-C(54)-C(53)	-0.7(12)

P(2)-C(49)-C(54)-C(53)	169.7(7)	C(52)-C(53)-C(54)-C(49)	1.0(14)