β-Diiminato complexes of arsenic including the formally As^{I} compound $[As_3L_3]$ $[L = \{N(C_6H_3Pr^{i}_2\text{-}2,6)C(H)\}_2CPh]$

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Supplementary Information:

The details of synthetic procedures and characterisation for compounds **1** and **2**; details of crystallographic data for **1** and **2**

*Synthesis of [AsI_2L] (**1**)*. KL (2.19 mmol, 22.5 mL of a 0.098 *M* solution in thf) was added dropwise to a solution of AsI_3 (1.00 g, 2.19 mmol) in thf (20 mL) under stirring at room temperature. The mixture was stirred for 2 d. The volatiles were removed *in vacuo*, and the residue was extracted with Et_2O. The dark-red extract was concentrated and stored at –15 °C yielding compound **1** (1.30 g, 1.50 mmol, 68%) as red crystals of **1**·(Et_2O). Anal. Calc. for $C_{37}H_{51}AsI_2N_2O$: C, 51.2; H, 5.92; N, 3.23. Found: C, 51.0, H, 5.69, N, 3.14%. ^{1}H-NMR (C_6D_6, 293 K): δ 1.11 (t, 6 H, Et_2O), 1.15 (d, 12 H, CH*Me*$_2$), 1.45 (d, 12 H, CH*Me*$_2$), 3.26 (q, 4 H, Et_2O), 3.65 (br s, 4 H, C*H*Me$_2$), 6.99 (d, 4 H, *m*-CH of Ar), 7.05-7.11 (m, 5 H, *p*-CH of Ar + CH of Ph), 7.20 (s, 2 H, NC*H*), 7.31 (m, 2 H, CH of Ph); ^{13}C-NMR (C_6D_6): δ 14.9 (Et_2O), 24.1 and 25.3 (CH*Me*$_2$), 29.7 and 31.3 (*C*HMe$_2$), 65.9 (Et_2O), 118.2 (*C*Ph), 124.5, 126.5, 128.6, 129.3, 130.5, 131.2, 135.9, 142.6 and 145.9 (Ar and Ph), 158.7 (NCH).

*Synthesis of [As_3L_3] (**2**)*. Et_2O (30 mL) was added to a mixture of compound **1** (0.81 g, 0.93 mmol) and KC_8 (0.249 g, 2.22 mmol) at room temperature. After stirring for 2 d the dark-brown mixture was filtered, the filtrate was concentrated, layered with hexane and stored at –15 °C for several days yielding black (dark brown in thin layer) crystals, which were washed with hexane (to remove a light-yellow crystalline co-product) and dried *in vacuo* to yield **2**·1.5(C_6H_{14}) (0.12 g, 0.22 mmol of As, 24%), mp 124-125 °C (decomp.). Anal. Calc. for $C_{108}H_{144}As_3N_6$: C, 74.1; H, 8.29; N, 4.80. Found: C, 74.0, H, 8.20, N, 4.83%. ^{1}H-NMR spectrum (C_6D_6, 293 K) showed broad signals in the aliphatic protons area (0.5 - 1.6 ppm), methine protons of Pr^i groups (2.6 - 3.8 ppm) and aromatic protons 6.6 - 8.2 ppm (including NCH of the ligand backbone); sharp Et_2O signals (as in **1**) were absent.

Table S1.1. Crystal data and structure refinement for [AsI_2(ArNCHCPhCHNAr)] . (Et_2O) (**1**).

Identification code	nov804	
Empirical formula	C37 H51 As I2 N2 O	
Formula weight	868.52	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$ (No.14)	
Unit cell dimensions	a = 11.2964(3) Å	α= 90°.
	b = 24.7180(4) Å	β= 97.267(1)°.
	c = 14.2829(4) Å	γ = 90°.
Volume	3956.10(17) $Å^3$	
Z	4	
Density (calculated)	1.46 Mg/m^3	
Absorption coefficient	2.45 mm^{-1}	
F(000)	1736	
Crystal size	0.15 x 0.15 x 0.05 mm^3	
Theta range for data collection	3.49 to 26.00°.	
Index ranges	-13<=h<=13, -30<=k<=30, -17<=l<=17	
Reflections collected	55518	
Independent reflections	7713 [R(int) = 0.062]	
Reflections with I>2sigma(I)	6182	
Completeness to theta = 26.00°	99.2 %	
Tmax. and Tmin.	0.785 and 0.605	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7713 / 0 / 388	
Goodness-of-fit on F^2	1.119	
Final R indices [I>2sigma(I)]	R1 = 0.047, wR2 = 0.100	
R indices (all data)	R1 = 0.066, wR2 = 0.107	
Largest diff. peak and hole	1.21 and -0.72 $e.Å^{-3}$	(near I)

Data collection KappaCCD , Program package WinGX , Abs correction MULTISCAN

Refinement using SHELXL-97 , Drawing using ORTEP-3 for Windows

Table S2.1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for nov804. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
As	12082(1)	1626(1)	5929(1)	33(1)
I(1)	9888(1)	959(1)	5678(1)	43(1)
I(2)	13903(1)	2383(1)	5944(1)	55(1)
O(1)	15693(6)	4080(3)	4399(6)	116(2)
N(1)	12315(3)	1474(2)	7259(3)	32(1)
N(2)	13008(3)	1009(2)	5645(3)	30(1)
C(1)	12360(4)	968(2)	7569(4)	34(1)
C(2)	12549(4)	511(2)	7023(4)	30(1)
C(3)	12981(4)	561(2)	6170(4)	30(1)
C(4)	12429(4)	-44(2)	7412(4)	35(1)
C(5)	11887(4)	-442(2)	6811(4)	38(1)
C(6)	11783(5)	-970(2)	7134(5)	51(2)
C(7)	12195(5)	-1097(2)	8059(5)	56(2)
C(8)	12713(7)	-706(3)	8654(5)	68(2)
C(9)	12834(6)	-183(2)	8337(4)	53(2)
C(10)	12460(4)	1919(2)	7934(4)	36(1)
C(11)	11520(5)	2271(2)	7990(4)	43(1)
C(12)	11694(6)	2695(2)	8633(5)	54(2)
C(13)	12768(6)	2766(2)	9191(5)	57(2)
C(14)	13699(6)	2409(2)	9134(4)	53(2)
C(15)	13561(5)	1974(2)	8500(4)	45(1)
C(16)	10321(5)	2226(2)	7382(4)	49(2)
C(17)	9293(6)	2193(3)	7975(6)	72(2)
C(18)	10142(7)	2694(3)	6671(5)	74(2)
C(19)	14610(5)	1585(3)	8500(5)	62(2)
C(20)	15799(6)	1873(4)	8504(7)	96(3)
C(21)	14685(7)	1200(3)	9331(6)	88(3)
C(22)	13765(4)	1027(2)	4894(4)	32(1)
C(23)	13236(4)	1082(2)	3966(4)	38(1)
C(24)	13973(5)	1069(2)	3256(4)	43(1)
C(25)	15199(5)	1002(2)	3473(4)	45(1)
C(26)	15698(5)	960(2)	4396(4)	41(1)

C(27)	15012(4)	978(2)	5139(4)	34(1)
C(28)	11897(5)	1139(2)	3691(4)	47(1)
C(29)	11410(5)	688(3)	3020(5)	70(2)
C(30)	11586(6)	1695(3)	3279(6)	77(2)
C(31)	15620(4)	949(2)	6142(4)	44(1)
C(32)	16639(5)	1358(3)	6329(5)	56(2)
C(33)	16112(6)	379(3)	6370(5)	68(2)
C(34)	15685(13)	3753(6)	5250(9)	143(5)
C(35)	16805(13)	3499(6)	5471(8)	146(5)
C(36)	14628(18)	4397(9)	4073(15)	263(14)
C(37)	14190(20)	4473(9)	3408(11)	263(13)

Table S3.1. Bond lengths [Å] and angles [°] for nov804.

As-N(1)	1.922(4)
As-N(2)	1.923(4)
As-I(2)	2.7781(6)
As-I(1)	2.9608(6)
O(1)-C(34)	1.460(13)
O(1)-C(36)	1.461(16)
N(1)-C(1)	1.326(6)
N(1)-C(10)	1.458(6)
N(2)-C(3)	1.340(6)
N(2)-C(22)	1.455(6)
C(1)-C(2)	1.403(7)
C(2)-C(3)	1.374(7)
C(2)-C(4)	1.493(6)
C(4)-C(9)	1.386(8)
C(4)-C(5)	1.395(7)
C(5)-C(6)	1.392(7)
C(6)-C(7)	1.380(9)
C(7)-C(8)	1.369(10)
C(8)-C(9)	1.383(8)
C(10)-C(11)	1.383(7)
C(10)-C(15)	1.401(7)
C(11)-C(12)	1.392(8)

C(11)-C(16)	1.517(8)
C(12)-C(13)	1.376(9)
C(13)-C(14)	1.384(9)
C(14)-C(15)	1.402(8)
C(15)-C(19)	1.526(8)
C(16)-C(17)	1.524(9)
C(16)-C(18)	1.537(9)
C(19)-C(21)	1.515(11)
C(19)-C(20)	1.519(10)
C(22)-C(23)	1.390(7)
C(22)-C(27)	1.413(7)
C(23)-C(24)	1.391(7)
C(23)-C(28)	1.521(7)
C(24)-C(25)	1.390(8)
C(25)-C(26)	1.371(8)
C(26)-C(27)	1.392(7)
C(27)-C(31)	1.510(8)
C(28)-C(30)	1.518(9)
C(28)-C(29)	1.528(9)
C(31)-C(32)	1.529(7)
C(31)-C(33)	1.535(8)
C(34)-C(35)	1.412(16)
C(36)-C(37)	1.033(18)

N(1)-As-N(2)	92.44(17)
N(1)-As-I(2)	96.66(12)
N(2)-As-I(2)	96.55(11)
N(1)-As-I(1)	91.05(12)
N(2)-As-I(1)	90.08(11)
I(2)-As-I(1)	169.59(2)
C(34)-O(1)-C(36)	118.1(14)
C(1)-N(1)-C(10)	119.6(4)
C(1)-N(1)-As	120.7(3)
C(10)-N(1)-As	119.7(3)
C(3)-N(2)-C(22)	119.7(4)
C(3)-N(2)-As	119.1(3)
C(22)-N(2)-As	121.2(3)

N(1)-C(1)-C(2)	125.1(5)
C(3)-C(2)-C(1)	121.1(4)
C(3)-C(2)-C(4)	118.1(4)
C(1)-C(2)-C(4)	120.4(5)
N(2)-C(3)-C(2)	127.3(4)
C(9)-C(4)-C(5)	118.5(5)
C(9)-C(4)-C(2)	123.2(5)
C(5)-C(4)-C(2)	118.3(5)
C(6)-C(5)-C(4)	120.4(6)
C(7)-C(6)-C(5)	119.9(6)
C(8)-C(7)-C(6)	119.9(5)
C(7)-C(8)-C(9)	120.6(6)
C(8)-C(9)-C(4)	120.6(6)
C(11)-C(10)-C(15)	122.5(5)
C(11)-C(10)-N(1)	119.3(4)
C(15)-C(10)-N(1)	118.2(4)
C(10)-C(11)-C(12)	117.9(5)
C(10)-C(11)-C(16)	123.9(5)
C(12)-C(11)-C(16)	118.3(5)
C(13)-C(12)-C(11)	121.2(6)
C(12)-C(13)-C(14)	120.4(5)
C(13)-C(14)-C(15)	120.3(6)
C(10)-C(15)-C(14)	117.7(5)
C(10)-C(15)-C(19)	124.9(5)
C(14)-C(15)-C(19)	117.4(5)
C(11)-C(16)-C(17)	112.0(5)
C(11)-C(16)-C(18)	110.8(5)
C(17)-C(16)-C(18)	111.2(5)
C(21)-C(19)-C(20)	109.3(6)
C(21)-C(19)-C(15)	111.2(6)
C(20)-C(19)-C(15)	113.0(6)
C(23)-C(22)-C(27)	122.6(5)
C(23)-C(22)-N(2)	119.0(4)
C(27)-C(22)-N(2)	118.4(5)
C(22)-C(23)-C(24)	117.9(5)
C(22)-C(23)-C(28)	123.3(5)
C(24)-C(23)-C(28)	118.8(5)

C(25)-C(24)-C(23)	120.8(5)
C(26)-C(25)-C(24)	120.0(5)
C(25)-C(26)-C(27)	122.0(5)
C(26)-C(27)-C(22)	116.6(5)
C(26)-C(27)-C(31)	119.4(4)
C(22)-C(27)-C(31)	124.0(5)
C(30)-C(28)-C(23)	111.0(5)
C(30)-C(28)-C(29)	111.8(6)
C(23)-C(28)-C(29)	111.2(5)
C(27)-C(31)-C(32)	112.1(5)
C(27)-C(31)-C(33)	110.6(5)
C(32)-C(31)-C(33)	109.0(5)
C(35)-C(34)-O(1)	109.5(10)
C(37)-C(36)-O(1)	132(2)

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Least-squares planes (x,y,z in crystal coordinates) and deviations from them
 (* indicates atom used to define plane)

  9.9869 (0.0254) x - 1.7642 (0.1844) y + 4.9464 (0.0527) z = 15.9169 (0.0153)

 *    0.0000 (0.0000)  C1
 *    0.0000 (0.0000)  C2
 *    0.0000 (0.0000)  C3

 Rms deviation of fitted atoms =   0.0000


  10.3893 (0.0070) x + 3.3183 (0.0711) y + 3.5658 (0.0275) z = 15.8668 (0.0070)

 Angle to previous plane (with approximate esd) = 13.12 ( 0.36 )

 *    0.0049 (0.0020)  N1
 *   -0.0048 (0.0020)  N2
 *   -0.0056 (0.0022)  C1
 *    0.0056 (0.0022)  C3
     -0.1547 (0.0067)  C2
     -0.6608 (0.0057)  As

 Rms deviation of fitted atoms =   0.0052


  9.2674 (0.0125) x + 13.9048 (0.0401) y - 0.0288 (0.0290) z = 13.4410 (0.0169)

 Angle to previous plane (with approximate esd) = 29.79 ( 0.20 )

 *    0.0000 (0.0000)  As
 *    0.0000 (0.0000)  N1
 *    0.0000 (0.0000)  N2
     -2.9603 (0.0006)  I1
      2.7395 (0.0012)  I2

 Rms deviation of fitted atoms =   0.0000
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Table S1.2. Crystal data and structure refinement for $[As_3(L)_3]$. 1.5(hexane) (**2**).

Identification code	dec3204	
Empirical formula	C99 H123 As3 N6 . 1.5(C6 H14)	
Formula weight	1751.05	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$ (No.2)	
Unit cell dimensions	a = 15.5396(4) Å	α= 101.334(2)°.
	b = 18.7915(4) Å	β= 96.248(1)°.
	c = 19.6985(5) Å	γ = 110.643(2)°.
Volume	5177.5(2) $Å^3$	
Z	2	
Density (calculated)	1.12 Mg/m^3	
Absorption coefficient	1.01 mm^{-1}	
F(000)	1866	
Crystal size	0.2 x 0.2 x 0.1 mm^3	
Theta range for data collection	3.45 to 26.70°.	
Index ranges	-18<=h<=19, -23<=k<=20, -24<=l<=24	
Reflections collected	67547	
Independent reflections	20830 [R(int) = 0.079]	
Reflections with I>2sigma(I)	13637	
Completeness to theta = 26.70°	95.0 %	
Tmax. and Tmin.	0.875 and 0.807	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	20830 / 15 / 1005	
Goodness-of-fit on F^2	1.122	
Final R indices [I>2sigma(I)]	R1 = 0.088, wR2 = 0.204	
R indices (all data)	R1 = 0.138, wR2 = 0.226	
Largest diff. peak and hole	1.05 and -0.57 $e.Å^{-3}$	

There is a clearly defined molecule of hexane solvate lying across an inversion centre. There is a second very poorly defined solvate molecule in a general position for which only five C atoms were resolved and which was included with SADI constraints. All solvate C atoms were left isotropic and H atoms were omitted. There is another area of small residual density (ca. 1e)which could not be resolved at all and was omitted from the model.

Data collection KappaCCD , Program package WinGX , Abs correction MULTISCAN

Refinement using SHELXL-97 , Drawing using ORTEP-3 for Windows

Table S2.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for dec3204. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
As(1)	5199(1)	2399(1)	1695(1)	34(1)
As(2)	5537(1)	3744(1)	2047(1)	33(1)
As(3)	6098(1)	2478(1)	2806(1)	30(1)
N(1)	5249(3)	3857(3)	1098(3)	33(1)
N(2)	4347(4)	3879(3)	2224(3)	39(1)
N(3)	5753(3)	1372(3)	2691(3)	31(1)
N(4)	5741(4)	-964(3)	2512(3)	41(1)
N(5)	7364(3)	2789(3)	2656(3)	31(1)
N(6)	9913(3)	4154(3)	2066(3)	39(1)
C(1)	4379(4)	3612(3)	743(3)	35(1)
C(2)	3552(4)	3404(4)	1012(3)	38(2)
C(3)	3588(4)	3601(4)	1728(4)	39(2)
C(4)	2652(4)	3101(4)	504(4)	46(2)
C(5)	2495(5)	2560(4)	-129(4)	54(2)
C(6)	1653(5)	2285(5)	-618(5)	64(2)
C(7)	953(6)	2554(6)	-457(5)	74(3)
C(8)	1091(6)	3083(5)	174(5)	72(2)
C(9)	1926(5)	3364(5)	643(5)	60(2)
C(10)	6021(4)	4090(3)	726(3)	34(1)
C(11)	6100(4)	3537(4)	172(3)	39(2)
C(12)	6838(5)	3810(4)	-176(4)	52(2)
C(13)	7465(5)	4577(4)	4(4)	57(2)
C(14)	7380(5)	5107(4)	556(4)	56(2)
C(15)	6653(5)	4874(4)	929(4)	43(2)
C(16)	5438(4)	2674(4)	-68(3)	40(2)
C(17)	4836(5)	2489(4)	-794(4)	50(2)
C(18)	5993(5)	2137(4)	-83(4)	51(2)
C(19)	6547(5)	5502(4)	1491(4)	49(2)
C(20)	7446(7)	5998(6)	2023(6)	105(4)
C(21)	6184(9)	6021(6)	1145(6)	102(4)
C(22)	4310(5)	4284(4)	2919(4)	45(2)
C(23)	4177(5)	3896(4)	3462(4)	49(2)

C(24)	4129(6)	4324(6)	4115(4)	64(2)
C(25)	4194(6)	5095(6)	4213(5)	68(2)
C(26)	4298(6)	5448(5)	3667(5)	69(2)
C(27)	4360(6)	5059(4)	3012(4)	58(2)
C(28)	4016(6)	3032(5)	3353(4)	59(2)
C(29)	2978(7)	2525(5)	3118(5)	85(3)
C(30)	4421(6)	2845(6)	4006(5)	80(3)
C(31)	4411(8)	5480(5)	2415(5)	83(3)
C(32)	5143(10)	6310(6)	2617(7)	127(5)
C(33)	3436(9)	5489(7)	2147(6)	107(4)
C(34)	6011(4)	931(3)	2173(3)	32(1)
C(35)	6018(4)	193(3)	2083(3)	33(1)
C(36)	5803(4)	-267(4)	2601(3)	38(1)
C(37)	6336(4)	-103(3)	1442(3)	38(2)
C(38)	7057(5)	-392(4)	1495(4)	48(2)
C(39)	7380(6)	-626(5)	907(5)	63(2)
C(40)	6993(7)	-620(5)	256(5)	71(2)
C(41)	6285(6)	-346(5)	187(4)	66(2)
C(42)	5957(5)	-101(4)	781(4)	48(2)
C(43)	5065(4)	1043(3)	3105(3)	35(1)
C(44)	5357(4)	1165(4)	3832(3)	37(1)
C(45)	4676(5)	896(4)	4225(4)	46(2)
C(46)	3747(5)	520(4)	3909(4)	54(2)
C(47)	3478(5)	394(4)	3198(4)	51(2)
C(48)	4126(4)	650(4)	2772(3)	38(2)
C(49)	6376(5)	1542(4)	4197(4)	47(2)
C(50)	6622(5)	2363(5)	4669(4)	59(2)
C(51)	6669(6)	1012(6)	4598(4)	72(2)
C(52)	3788(4)	472(4)	1981(4)	44(2)
C(53)	3503(6)	-399(4)	1631(4)	60(2)
C(54)	2980(5)	738(5)	1803(5)	65(2)
C(55)	5588(5)	-1330(4)	3082(4)	46(2)
C(56)	4680(6)	-1698(4)	3197(4)	55(2)
C(57)	4566(6)	-2093(5)	3728(4)	65(2)
C(58)	5325(7)	-2114(5)	4139(4)	68(2)
C(59)	6215(7)	-1741(5)	4031(4)	65(2)
C(60)	6379(6)	-1353(4)	3497(4)	56(2)

C(61)	3831(6)	-1683(6)	2754(5)	71(3)
C(62)	3410(9)	-2393(10)	2144(6)	143(6)
C(63)	3089(6)	-1612(5)	3159(5)	76(3)
C(64)	7327(6)	-996(5)	3339(5)	72(3)
C(65)	8102(8)	-649(7)	3987(7)	123(5)
C(66)	7490(7)	-1584(6)	2766(6)	99(4)
C(67)	7586(4)	2717(3)	1999(3)	32(1)
C(68)	8391(4)	3098(4)	1785(3)	35(1)
C(69)	9139(4)	3794(3)	2237(3)	35(1)
C(70)	8455(4)	2786(4)	1044(3)	37(1)
C(71)	8248(4)	1980(4)	788(4)	42(2)
C(72)	8252(5)	1684(4)	88(4)	51(2)
C(73)	8463(5)	2169(5)	-367(4)	54(2)
C(74)	8673(4)	2958(5)	-113(4)	50(2)
C(75)	8681(4)	3270(4)	584(4)	42(2)
C(76)	8044(4)	3073(3)	3309(3)	34(1)
C(77)	8527(4)	2601(4)	3480(4)	39(2)
C(78)	9114(5)	2868(4)	4139(4)	50(2)
C(79)	9226(5)	3544(4)	4609(4)	50(2)
C(80)	8776(4)	4020(4)	4426(4)	44(2)
C(81)	8184(4)	3798(4)	3769(3)	38(1)
C(82)	8451(4)	1842(4)	2980(4)	44(2)
C(83)	9321(5)	1969(4)	2641(4)	55(2)
C(84)	8302(6)	1159(5)	3319(5)	66(2)
C(85)	7759(5)	4358(4)	3571(4)	43(2)
C(86)	7040(5)	4446(4)	4017(4)	56(2)
C(87)	8509(6)	5173(4)	3642(4)	62(2)
C(88)	10541(4)	4863(4)	2571(3)	40(2)
C(89)	11080(4)	4821(4)	3174(3)	44(2)
C(90)	11678(5)	5526(5)	3642(4)	57(2)
C(91)	11735(6)	6244(5)	3521(4)	68(2)
C(92)	11224(5)	6260(4)	2916(4)	58(2)
C(93)	10629(5)	5577(4)	2424(4)	47(2)
C(94)	11042(4)	4031(4)	3281(4)	47(2)
C(95)	11498(5)	3668(5)	2739(4)	62(2)
C(96)	11470(5)	4060(5)	4020(4)	61(2)
C(97)	10106(5)	5590(4)	1733(4)	54(2)

C(98)	10040(6)	6378(5)	1723(5)	72(2)
C(99)	10571(6)	5347(5)	1126(4)	66(2)
C(1S)	10375(9)	304(8)	275(7)	130(5)
C(2S)	10211(11)	907(9)	759(8)	165(6)
C(3S)	10971(9)	1524(7)	1300(7)	121(4)
C(4S)	7240(20)	6742(18)	4578(16)	285(13)
C(5S)	8010(30)	7090(20)	4200(20)	357(18)
C(6S)	9020(30)	7560(20)	4540(20)	337(17)
C(7S)	9590(30)	7590(20)	3960(20)	354(18)
C(8S)	10620(30)	8080(20)	4102(17)	308(15)

Table S3.2. Bond lengths [Å] and angles [°] for dec3204.

As(1)-As(2)	2.3328(8)
As(1)-As(3)	2.4139(9)
As(2)-N(1)	1.944(5)
As(2)-N(2)	2.010(5)
As(3)-N(3)	1.912(5)
As(3)-N(5)	1.919(4)
N(1)-C(1)	1.326(7)
N(1)-C(10)	1.454(7)
N(2)-C(3)	1.317(8)
N(2)-C(22)	1.448(8)
N(3)-C(34)	1.372(7)
N(3)-C(43)	1.452(7)
N(4)-C(36)	1.255(8)
N(4)-C(55)	1.428(8)
N(5)-C(67)	1.368(7)
N(5)-C(76)	1.445(7)
N(6)-C(69)	1.274(7)
N(6)-C(88)	1.438(8)
C(1)-C(2)	1.399(8)
C(2)-C(3)	1.375(9)
C(2)-C(4)	1.482(9)
C(4)-C(5)	1.382(10)
C(4)-C(9)	1.413(9)
C(5)-C(6)	1.400(10)
C(6)-C(7)	1.392(11)
C(7)-C(8)	1.373(12)
C(8)-C(9)	1.372(11)
C(10)-C(11)	1.399(9)
C(10)-C(15)	1.399(9)
C(11)-C(12)	1.394(9)
C(11)-C(16)	1.525(9)
C(12)-C(13)	1.373(10)
C(13)-C(14)	1.374(10)
C(14)-C(15)	1.404(9)
C(15)-C(19)	1.519(9)

C(16)-C(17)	1.526(9)
C(16)-C(18)	1.540(9)
C(19)-C(21)	1.515(10)
C(19)-C(20)	1.516(11)
C(22)-C(23)	1.402(10)
C(22)-C(27)	1.405(10)
C(23)-C(24)	1.402(10)
C(23)-C(28)	1.520(10)
C(24)-C(25)	1.389(12)
C(25)-C(26)	1.366(12)
C(26)-C(27)	1.383(11)
C(27)-C(31)	1.535(12)
C(28)-C(29)	1.518(12)
C(28)-C(30)	1.526(11)
C(31)-C(32)	1.514(13)
C(31)-C(33)	1.558(15)
C(34)-C(35)	1.367(8)
C(35)-C(36)	1.455(8)
C(35)-C(37)	1.483(9)
C(37)-C(42)	1.371(9)
C(37)-C(38)	1.410(9)
C(38)-C(39)	1.367(10)
C(39)-C(40)	1.359(12)
C(40)-C(41)	1.374(11)
C(41)-C(42)	1.386(10)
C(43)-C(48)	1.396(8)
C(43)-C(44)	1.402(9)
C(44)-C(45)	1.390(9)
C(44)-C(49)	1.513(9)
C(45)-C(46)	1.373(10)
C(46)-C(47)	1.366(10)
C(47)-C(48)	1.396(9)
C(48)-C(52)	1.520(9)
C(49)-C(50)	1.527(10)
C(49)-C(51)	1.541(10)
C(52)-C(53)	1.527(10)
C(52)-C(54)	1.537(9)

C(55)-C(56)	1.402(10)
C(55)-C(60)	1.418(10)
C(56)-C(57)	1.389(10)
C(56)-C(61)	1.512(11)
C(57)-C(58)	1.374(12)
C(58)-C(59)	1.375(12)
C(59)-C(60)	1.390(11)
C(60)-C(64)	1.483(12)
C(61)-C(62)	1.495(15)
C(61)-C(63)	1.500(11)
C(64)-C(65)	1.512(13)
C(64)-C(66)	1.526(13)
C(67)-C(68)	1.363(8)
C(68)-C(69)	1.449(8)
C(68)-C(70)	1.490(9)
C(70)-C(75)	1.392(9)
C(70)-C(71)	1.405(9)
C(71)-C(72)	1.384(9)
C(72)-C(73)	1.384(10)
C(73)-C(74)	1.373(10)
C(74)-C(75)	1.379(9)
C(76)-C(81)	1.409(9)
C(76)-C(77)	1.412(8)
C(77)-C(78)	1.390(9)
C(77)-C(82)	1.524(9)
C(78)-C(79)	1.360(10)
C(79)-C(80)	1.389(10)
C(80)-C(81)	1.399(9)
C(81)-C(85)	1.513(9)
C(82)-C(84)	1.520(10)
C(82)-C(83)	1.538(9)
C(85)-C(86)	1.528(9)
C(85)-C(87)	1.532(9)
C(88)-C(93)	1.390(9)
C(88)-C(89)	1.410(9)
C(89)-C(90)	1.391(9)
C(89)-C(94)	1.522(10)

C(90)-C(91)	1.389(11)
C(91)-C(92)	1.370(11)
C(92)-C(93)	1.386(9)
C(93)-C(97)	1.517(10)
C(94)-C(96)	1.517(10)
C(94)-C(95)	1.524(10)
C(97)-C(98)	1.524(10)
C(97)-C(99)	1.539(11)

As(2)-As(1)-As(3)	89.88(3)
N(1)-As(2)-N(2)	88.2(2)
N(1)-As(2)-As(1)	95.13(14)
N(2)-As(2)-As(1)	107.64(15)
N(3)-As(3)-N(5)	101.2(2)
N(3)-As(3)-As(1)	96.97(14)
N(5)-As(3)-As(1)	104.14(15)
C(1)-N(1)-C(10)	118.9(5)
C(1)-N(1)-As(2)	122.7(4)
C(10)-N(1)-As(2)	117.5(4)
C(3)-N(2)-C(22)	118.3(5)
C(3)-N(2)-As(2)	122.1(4)
C(22)-N(2)-As(2)	119.6(4)
C(34)-N(3)-C(43)	124.1(5)
C(34)-N(3)-As(3)	121.5(4)
C(43)-N(3)-As(3)	113.4(4)
C(36)-N(4)-C(55)	118.9(5)
C(67)-N(5)-C(76)	124.4(5)
C(67)-N(5)-As(3)	123.0(4)
C(76)-N(5)-As(3)	112.5(4)
C(69)-N(6)-C(88)	115.9(5)
N(1)-C(1)-C(2)	127.4(6)
C(3)-C(2)-C(1)	120.2(6)
C(3)-C(2)-C(4)	121.2(6)
C(1)-C(2)-C(4)	117.6(6)
N(2)-C(3)-C(2)	126.2(6)
C(5)-C(4)-C(9)	117.5(7)
C(5)-C(4)-C(2)	121.2(6)

C(9)-C(4)-C(2)	121.2(7)
C(4)-C(5)-C(6)	121.5(7)
C(7)-C(6)-C(5)	119.2(8)
C(8)-C(7)-C(6)	120.1(8)
C(9)-C(8)-C(7)	120.4(8)
C(8)-C(9)-C(4)	121.2(8)
C(11)-C(10)-C(15)	122.2(6)
C(11)-C(10)-N(1)	119.7(5)
C(15)-C(10)-N(1)	118.0(5)
C(12)-C(11)-C(10)	116.4(6)
C(12)-C(11)-C(16)	119.2(6)
C(10)-C(11)-C(16)	124.4(6)
C(13)-C(12)-C(11)	123.1(7)
C(12)-C(13)-C(14)	119.5(7)
C(13)-C(14)-C(15)	120.6(7)
C(10)-C(15)-C(14)	118.2(6)
C(10)-C(15)-C(19)	123.6(6)
C(14)-C(15)-C(19)	118.0(6)
C(11)-C(16)-C(17)	111.4(5)
C(11)-C(16)-C(18)	110.6(5)
C(17)-C(16)-C(18)	109.7(5)
C(21)-C(19)-C(20)	110.3(8)
C(21)-C(19)-C(15)	109.9(7)
C(20)-C(19)-C(15)	113.2(7)
C(23)-C(22)-C(27)	122.0(6)
C(23)-C(22)-N(2)	120.5(6)
C(27)-C(22)-N(2)	117.4(6)
C(24)-C(23)-C(22)	117.1(7)
C(24)-C(23)-C(28)	119.8(7)
C(22)-C(23)-C(28)	123.0(6)
C(25)-C(24)-C(23)	121.2(8)
C(26)-C(25)-C(24)	120.2(8)
C(25)-C(26)-C(27)	121.4(8)
C(26)-C(27)-C(22)	118.2(7)
C(26)-C(27)-C(31)	118.0(7)
C(22)-C(27)-C(31)	123.7(7)
C(29)-C(28)-C(23)	110.3(6)

C(29)-C(28)-C(30)	110.2(7)
C(23)-C(28)-C(30)	113.1(7)
C(32)-C(31)-C(27)	113.8(9)
C(32)-C(31)-C(33)	109.5(9)
C(27)-C(31)-C(33)	110.3(8)
C(35)-C(34)-N(3)	131.2(6)
C(34)-C(35)-C(36)	123.4(6)
C(34)-C(35)-C(37)	116.0(5)
C(36)-C(35)-C(37)	120.4(5)
N(4)-C(36)-C(35)	124.6(6)
C(42)-C(37)-C(38)	117.2(6)
C(42)-C(37)-C(35)	122.2(6)
C(38)-C(37)-C(35)	120.6(6)
C(39)-C(38)-C(37)	120.3(7)
C(40)-C(39)-C(38)	121.5(8)
C(39)-C(40)-C(41)	119.6(8)
C(40)-C(41)-C(42)	119.4(8)
C(37)-C(42)-C(41)	122.0(7)
C(48)-C(43)-C(44)	121.9(6)
C(48)-C(43)-N(3)	118.9(5)
C(44)-C(43)-N(3)	119.1(5)
C(45)-C(44)-C(43)	118.1(6)
C(45)-C(44)-C(49)	118.9(6)
C(43)-C(44)-C(49)	123.0(6)
C(46)-C(45)-C(44)	120.8(7)
C(47)-C(46)-C(45)	120.3(6)
C(46)-C(47)-C(48)	121.7(6)
C(43)-C(48)-C(47)	117.1(6)
C(43)-C(48)-C(52)	123.5(5)
C(47)-C(48)-C(52)	119.4(6)
C(44)-C(49)-C(50)	112.1(6)
C(44)-C(49)-C(51)	112.3(6)
C(50)-C(49)-C(51)	111.9(6)
C(48)-C(52)-C(53)	111.1(5)
C(48)-C(52)-C(54)	112.1(6)
C(53)-C(52)-C(54)	110.5(6)
C(56)-C(55)-C(60)	121.3(6)

C(56)-C(55)-N(4)	120.9(6)
C(60)-C(55)-N(4)	117.7(6)
C(57)-C(56)-C(55)	118.5(7)
C(57)-C(56)-C(61)	119.8(7)
C(55)-C(56)-C(61)	121.8(6)
C(58)-C(57)-C(56)	120.9(8)
C(57)-C(58)-C(59)	120.3(7)
C(58)-C(59)-C(60)	121.9(8)
C(59)-C(60)-C(55)	117.1(8)
C(59)-C(60)-C(64)	122.6(8)
C(55)-C(60)-C(64)	120.3(7)
C(62)-C(61)-C(63)	109.4(8)
C(62)-C(61)-C(56)	110.9(8)
C(63)-C(61)-C(56)	114.1(7)
C(60)-C(64)-C(65)	113.7(9)
C(60)-C(64)-C(66)	109.8(7)
C(65)-C(64)-C(66)	113.2(9)
C(68)-C(67)-N(5)	130.7(6)
C(67)-C(68)-C(69)	122.4(6)
C(67)-C(68)-C(70)	116.8(5)
C(69)-C(68)-C(70)	120.7(5)
N(6)-C(69)-C(68)	124.5(6)
C(75)-C(70)-C(71)	118.5(6)
C(75)-C(70)-C(68)	121.7(6)
C(71)-C(70)-C(68)	119.8(6)
C(72)-C(71)-C(70)	119.7(6)
C(71)-C(72)-C(73)	121.2(7)
C(74)-C(73)-C(72)	119.0(7)
C(73)-C(74)-C(75)	121.1(7)
C(74)-C(75)-C(70)	120.6(6)
C(81)-C(76)-C(77)	121.7(6)
C(81)-C(76)-N(5)	119.4(5)
C(77)-C(76)-N(5)	118.9(5)
C(78)-C(77)-C(76)	116.7(6)
C(78)-C(77)-C(82)	119.6(6)
C(76)-C(77)-C(82)	123.6(6)
C(79)-C(78)-C(77)	122.9(7)

C(78)-C(79)-C(80)	120.0(6)
C(79)-C(80)-C(81)	120.5(6)
C(80)-C(81)-C(76)	118.0(6)
C(80)-C(81)-C(85)	118.8(6)
C(76)-C(81)-C(85)	123.1(6)
C(84)-C(82)-C(77)	114.3(6)
C(84)-C(82)-C(83)	108.7(6)
C(77)-C(82)-C(83)	111.1(5)
C(81)-C(85)-C(86)	112.1(6)
C(81)-C(85)-C(87)	111.8(6)
C(86)-C(85)-C(87)	108.8(6)
C(93)-C(88)-C(89)	121.9(6)
C(93)-C(88)-N(6)	118.0(6)
C(89)-C(88)-N(6)	120.0(6)
C(90)-C(89)-C(88)	117.5(7)
C(90)-C(89)-C(94)	121.8(7)
C(88)-C(89)-C(94)	120.6(6)
C(91)-C(90)-C(89)	121.1(7)
C(92)-C(91)-C(90)	119.6(7)
C(91)-C(92)-C(93)	121.8(7)
C(92)-C(93)-C(88)	117.9(7)
C(92)-C(93)-C(97)	122.0(7)
C(88)-C(93)-C(97)	120.0(6)
C(96)-C(94)-C(89)	114.4(6)
C(96)-C(94)-C(95)	110.3(6)
C(89)-C(94)-C(95)	110.0(6)
C(93)-C(97)-C(98)	114.4(7)
C(93)-C(97)-C(99)	109.4(6)
C(98)-C(97)-C(99)	109.6(6)