Table 1. Crystal data and structure refinement for DAV12 (CCDC 161166).

Empirical formula	$C_{42}H_{46}N_4PtCl_2 \bullet 3(C_3H_7NO)\ 2(H_2O)$
Formula weight	1128.14
Crystallization Solvent	DMF/ether
Crystal Habit	Irregular plate
Crystal size	0.30 x 0.19 x 0.07 mm^3
Crystal color	Yellow

Data Collection

Preliminary Photos	Rotation	
Type of diffractometer	CCD area detector	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	98(2) K	
θ range for 19064 reflections used in lattice determination	2.17 to 27.84°	
Unit cell dimensions	a = 12.3592(9) Å b = 15.0644(11) Å c = 15.0726(11) Å	α= 91.0060(10)° β= 105.7790(10)° γ = 112.0910(10)°
Volume	2479.6(3) $Å^3$	
Z	2	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	1.511 Mg/m^3	
F(000)	1156	
Data collection program	Bruker SMART	
θ range for data collection	1.47 to 28.43°	
Completeness to θ = 28.43°	91.7 %	
Index ranges	$-16 \le h \le 16, -19 \le k \le 19, -20 \le l \le 19$	
Data collection scan type	ω scans at 7 ϕ settings	
Data reduction program	Bruker SAINT v6.2	
Reflections collected	51207	
Independent reflections	11473 [R_{int}= 0.0571]	
Absorption coefficient	2.991 mm^{-1}	
Absorption correction	SADABS	
Max. and min. transmission	1.000000 and 0.822175	

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Patterson method
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	11473 / 0 / 611
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.441
Final R indices [$I>2\sigma(I)$, 9227 reflections]	R1 = 0.0391, *w*R2 = 0.0634
R indices (all data)	R1 = 0.0552, *w*R2 = 0.0648
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.001
Average shift/error	0.000
Largest diff. peak and hole	2.338 and -2.085 e.Å^{-3}

Special Refinement Details

This structure includes three molecules of dimethylformamide and two water molecules in addition to the to the platinum complex and its chloride counter ions. The water molecules are hydrogen bonded as indicated in Table 7. The hydrogen atoms of the water molecules were fixed during least squares refinement, all other hydrogen atoms were constrained to ride the atoms to which they are bonded.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for DAV12 (CCDC 161166). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Pt	9366(1)	9447(1)	6970(1)	21(1)
Cl(1)	7411(1)	5530(1)	9589(1)	46(1)
Cl(2)	7767(1)	4359(1)	6147(1)	72(1)
N(1)	8479(3)	10291(3)	6273(2)	25(1)
N(2)	7706(3)	8379(3)	6146(2)	25(1)
N(3)	14246(3)	13185(2)	8746(2)	25(1)
N(4)	10918(3)	6158(2)	8726(2)	25(1)
C(1)	7425(4)	9772(3)	5592(3)	28(1)
C(2)	7000(4)	8736(3)	5519(3)	28(1)
C(3)	8845(4)	11250(3)	6421(3)	31(1)
C(4)	8207(4)	11732(4)	5872(3)	39(1)
C(5)	7196(4)	11231(4)	5155(3)	39(1)
C(6)	6771(4)	10235(4)	4991(3)	34(1)
C(7)	5672(4)	9620(4)	4256(3)	39(1)
C(8)	5023(4)	10045(4)	3617(3)	48(2)
C(9)	3961(5)	9496(5)	2920(3)	55(2)
C(10)	3282(5)	9920(5)	2292(3)	64(2)
C(11)	2260(6)	9386(7)	1634(4)	80(2)
C(12)	1803(5)	8390(6)	1538(3)	64(2)
C(13)	2426(5)	7893(5)	2128(3)	75(2)
C(14)	3537(4)	8491(5)	2837(3)	56(2)
C(15)	4185(4)	8026(4)	3470(3)	50(2)
C(16)	5237(4)	8598(4)	4173(3)	40(1)
C(17)	5914(4)	8144(4)	4843(3)	33(1)
C(18)	5566(4)	7157(4)	4834(3)	42(1)
C(19)	6266(4)	6784(4)	5467(3)	43(1)
C(20)	7343(4)	7430(4)	6115(3)	34(1)
C(21)	10951(3)	10590(3)	7594(3)	19(1)
C(22)	11630(3)	11162(3)	7033(3)	20(1)
C(23)	12687(3)	11983(3)	7421(3)	23(1)
C(24)	13102(3)	12277(3)	8367(3)	22(1)
C(25)	12482(4)	11758(3)	8931(3)	24(1)
C(26)	11415(3)	10919(3)	8559(3)	20(1)
C(27)	11215(4)	10911(3)	5981(2)	27(1)
C(28)	10776(4)	10399(3)	9227(2)	27(1)
C(29)	14068(4)	14027(3)	8319(3)	42(1)
C(30)	14600(4)	13430(3)	9781(3)	34(1)
C(31)	15306(4)	13059(3)	8531(3)	38(1)
C(32)	9987(3)	8475(3)	7576(2)	19(1)
C(33)	10897(3)	8243(3)	7350(2)	19(1)
C(34)	11199(3)	7496(3)	7715(3)	23(1)
C(35)	10621(3)	6964(3)	8313(3)	21(1)
C(36)	9740(3)	7184(3)	8559(3)	23(1)
C(37)	9415(3)	7922(3)	8187(3)	20(1)
C(38)	11539(3)	8763(3)	6685(3)	25(1)
C(39)	8371(3)	8050(3)	8439(3)	25(1)
C(40)	11454(4)	6411(3)	9760(3)	33(1)

C(41)	11826(4)	5949(3)	8358(3)	34(1)
C(42)	9779(4)	5247(3)	8497(3)	32(1)
N(61)	4137(3)	6344(3)	6810(2)	35(1)
O(61)	3910(4)	7760(3)	6752(2)	81(1)
C(61)	3778(4)	6992(4)	6382(3)	46(1)
C(62)	4733(4)	6505(3)	7801(3)	40(1)
C(63)	3867(5)	5411(4)	6321(3)	56(2)
N(71)	9522(3)	6288(3)	4593(3)	44(1)
O(71)	8604(4)	6142(3)	3036(3)	80(1)
C(71)	9396(5)	6068(4)	3697(4)	53(2)
C(72)	8726(4)	6646(4)	4902(4)	63(2)
C(73)	10514(4)	6213(3)	5329(3)	43(1)
N(81)	3807(3)	9416(2)	9053(2)	21(1)
O(81)	4106(2)	8033(2)	9340(2)	31(1)
C(81)	4230(3)	8750(3)	8933(3)	26(1)
C(82)	3083(4)	9321(3)	9689(3)	28(1)
C(83)	4026(4)	10256(3)	8563(3)	28(1)
O(91)	6541(4)	5235(4)	7297(3)	104(2)
O(92)	9411(4)	6663(4)	1407(4)	126(2)

Table 3. Selected bond lengths [Å] and angles [°] for DAV12 (CCDC 161166).

Pt-C(32)	2.020(4)	C(32)-Pt-C(21)	93.69(15)
Pt-C(21)	2.023(4)	C(32)-Pt-N(1)	171.86(15)
Pt-N(1)	2.095(3)	C(21)-Pt-N(1)	94.37(14)
Pt-N(2)	2.098(3)	C(32)-Pt-N(2)	93.47(14)
		C(21)-Pt-N(2)	171.15(14)
		N(1)-Pt-N(2)	78.61(14)

Table 4. Bond lengths [Å] and angles [°] for DAV12 (CCDC 161166).

Pt-C(32)	2.020(4)	C(21)-C(22)	1.424(5)
Pt-C(21)	2.023(4)	C(22)-C(23)	1.386(5)
Pt-N(1)	2.095(3)	C(22)-C(27)	1.520(5)
Pt-N(2)	2.098(3)	C(23)-C(24)	1.379(5)
N(1)-C(3)	1.335(5)	C(23)-H(23)	0.9500
N(1)-C(1)	1.357(5)	C(24)-C(25)	1.359(5)
N(2)-C(20)	1.324(5)	C(25)-C(26)	1.403(5)
N(2)-C(2)	1.365(5)	C(25)-H(25)	0.9500
N(3)-C(29)	1.493(5)	C(26)-C(28)	1.499(5)
N(3)-C(30)	1.500(5)	C(27)-H(27A)	0.9800
N(3)-C(24)	1.509(5)	C(27)-H(27B)	0.9800
N(3)-C(31)	1.508(5)	C(27)-H(27C)	0.9800
N(4)-C(35)	1.495(5)	C(28)-H(28A)	0.9800
N(4)-C(40)	1.497(5)	C(28)-H(28B)	0.9800
N(4)-C(42)	1.500(5)	C(28)-H(28C)	0.9800
N(4)-C(41)	1.504(5)	C(29)-H(29A)	0.9800
C(1)-C(6)	1.418(5)	C(29)-H(29B)	0.9800
C(1)-C(2)	1.439(6)	C(29)-H(29C)	0.9800
C(2)-C(17)	1.399(6)	C(30)-H(30A)	0.9800
C(3)-C(4)	1.390(5)	C(30)-H(30B)	0.9800
C(3)-H(3)	0.9500	C(30)-H(30C)	0.9800
C(4)-C(5)	1.352(6)	C(31)-H(31A)	0.9800
C(4)-H(4)	0.9500	C(31)-H(31B)	0.9800
C(5)-C(6)	1.382(6)	C(31)-H(31C)	0.9800
C(5)-H(5)	0.9500	C(32)-C(37)	1.407(5)
C(6)-C(7)	1.459(6)	C(32)-C(33)	1.415(5)
C(7)-C(8)	1.403(6)	C(33)-C(34)	1.390(5)
C(7)-C(16)	1.418(7)	C(33)-C(38)	1.497(5)
C(8)-C(9)	1.383(7)	C(34)-C(35)	1.383(5)
C(8)-H(8)	0.9500	C(34)-H(34)	0.9500
C(9)-C(14)	1.394(8)	C(35)-C(36)	1.386(5)
C(9)-C(10)	1.415(6)	C(36)-C(37)	1.395(5)
C(10)-C(11)	1.324(8)	C(36)-H(36)	0.9500
C(10)-H(10)	0.9500	C(37)-C(39)	1.515(5)
C(11)-C(12)	1.378(8)	C(38)-H(38A)	0.9800
C(11)-H(11)	0.9500	C(38)-H(38B)	0.9800
C(12)-C(13)	1.424(7)	C(38)-H(38C)	0.9800
C(12)-H(12)	0.9500	C(39)-H(39A)	0.9800
C(13)-C(14)	1.441(7)	C(39)-H(39B)	0.9800
C(13)-H(13)	0.9500	C(39)-H(39C)	0.9800
C(14)-C(15)	1.439(7)	C(40)-H(40A)	0.9800
C(15)-C(16)	1.390(6)	C(40)-H(40B)	0.9800
C(15)-H(15)	0.9500	C(40)-H(40C)	0.9800
C(16)-C(17)	1.477(6)	C(41)-H(41A)	0.9800
C(17)-C(18)	1.383(6)	C(41)-H(41B)	0.9800
C(18)-C(19)	1.382(6)	C(41)-H(41C)	0.9800
C(18)-H(18)	0.9500	C(42)-H(42A)	0.9800
C(19)-C(20)	1.399(6)	C(42)-H(42B)	0.9800
C(19)-H(19)	0.9500	C(42)-H(42C)	0.9800
C(20)-H(20)	0.9500	N(61)-C(61)	1.326(5)
C(21)-C(26)	1.413(5)	N(61)-C(62)	1.445(5)

N(61)-C(63)	1.452(6)	C(35)-N(4)-C(40)	109.9(3)
O(61)-C(61)	1.210(5)	C(35)-N(4)-C(42)	109.9(3)
C(61)-H(61)	0.9500	C(40)-N(4)-C(42)	109.6(3)
C(62)-H(62A)	0.9800	C(35)-N(4)-C(41)	112.5(3)
C(62)-H(62B)	0.9800	C(40)-N(4)-C(41)	107.8(3)
C(62)-H(62C)	0.9800	C(42)-N(4)-C(41)	107.2(3)
C(63)-H(63A)	0.9800	N(1)-C(1)-C(6)	121.2(4)
C(63)-H(63B)	0.9800	N(1)-C(1)-C(2)	116.9(4)
C(63)-H(63C)	0.9800	C(6)-C(1)-C(2)	121.9(4)
N(71)-C(71)	1.338(6)	N(2)-C(2)-C(17)	123.0(4)
N(71)-C(73)	1.454(5)	N(2)-C(2)-C(1)	116.3(4)
N(71)-C(72)	1.455(6)	C(17)-C(2)-C(1)	120.7(4)
O(71)-C(71)	1.231(5)	N(1)-C(3)-C(4)	121.9(4)
C(71)-H(71)	0.9500	N(1)-C(3)-H(3)	119.0
C(72)-H(72A)	0.9800	C(4)-C(3)-H(3)	119.0
C(72)-H(72B)	0.9800	C(5)-C(4)-C(3)	119.9(5)
C(72)-H(72C)	0.9800	C(5)-C(4)-H(4)	120.0
C(73)-H(73A)	0.9800	C(3)-C(4)-H(4)	120.0
C(73)-H(73B)	0.9800	C(4)-C(5)-C(6)	120.0(4)
C(73)-H(73C)	0.9800	C(4)-C(5)-H(5)	120.0
N(81)-C(81)	1.325(5)	C(6)-C(5)-H(5)	120.0
N(81)-C(83)	1.450(5)	C(5)-C(6)-C(1)	118.0(4)
N(81)-C(82)	1.454(5)	C(5)-C(6)-C(7)	124.6(4)
O(81)-C(81)	1.231(4)	C(1)-C(6)-C(7)	117.4(5)
C(81)-H(81)	0.9500	C(8)-C(7)-C(16)	118.9(5)
C(82)-H(82A)	0.9800	C(8)-C(7)-C(6)	119.5(5)
C(82)-H(82B)	0.9800	C(16)-C(7)-C(6)	121.5(4)
C(82)-H(82C)	0.9800	C(9)-C(8)-C(7)	121.9(6)
C(83)-H(83A)	0.9800	C(9)-C(8)-H(8)	119.1
C(83)-H(83B)	0.9800	C(7)-C(8)-H(8)	119.1
C(83)-H(83C)	0.9800	C(8)-C(9)-C(14)	119.2(5)
O(91)-H(91A)	1.0662	C(8)-C(9)-C(10)	122.2(6)
O(91)-H(91B)	0.8946	C(14)-C(9)-C(10)	118.7(6)
O(92)-H(92A)	0.8812	C(11)-C(10)-C(9)	121.6(7)
O(92)-H(92B)	0.8914	C(11)-C(10)-H(10)	119.2
		C(9)-C(10)-H(10)	119.2
C(32)-Pt-C(21)	93.69(15)	C(10)-C(11)-C(12)	121.4(7)
C(32)-Pt-N(1)	171.86(15)	C(10)-C(11)-H(11)	119.3
C(21)-Pt-N(1)	94.37(14)	C(12)-C(11)-H(11)	119.3
C(32)-Pt-N(2)	93.47(14)	C(11)-C(12)-C(13)	121.4(6)
C(21)-Pt-N(2)	171.15(14)	C(11)-C(12)-H(12)	119.3
N(1)-Pt-N(2)	78.61(14)	C(13)-C(12)-H(12)	119.3
C(3)-N(1)-C(1)	118.8(4)	C(12)-C(13)-C(14)	116.1(6)
C(3)-N(1)-Pt	127.5(3)	C(12)-C(13)-H(13)	121.9
C(1)-N(1)-Pt	113.7(3)	C(14)-C(13)-H(13)	121.9
C(20)-N(2)-C(2)	118.5(4)	C(9)-C(14)-C(15)	120.7(5)
C(20)-N(2)-Pt	127.6(3)	C(9)-C(14)-C(13)	120.8(5)
C(2)-N(2)-Pt	113.6(3)	C(15)-C(14)-C(13)	118.4(6)
C(29)-N(3)-C(30)	107.5(3)	C(16)-C(15)-C(14)	118.8(5)
C(29)-N(3)-C(24)	110.3(3)	C(16)-C(15)-H(15)	120.6
C(30)-N(3)-C(24)	113.0(3)	C(14)-C(15)-H(15)	120.6
C(29)-N(3)-C(31)	109.4(3)	C(15)-C(16)-C(7)	120.5(5)
C(30)-N(3)-C(31)	107.0(3)	C(15)-C(16)-C(17)	120.2(5)
C(24)-N(3)-C(31)	109.6(3)	C(7)-C(16)-C(17)	119.3(4)

C(18)-C(17)-C(2)	116.8(4)	N(3)-C(31)-H(31A)	109.5
C(18)-C(17)-C(16)	124.1(4)	N(3)-C(31)-H(31B)	109.5
C(2)-C(17)-C(16)	119.1(5)	H(31A)-C(31)-H(31B)	109.5
C(17)-C(18)-C(19)	121.0(4)	N(3)-C(31)-H(31C)	109.5
C(17)-C(18)-H(18)	119.5	H(31A)-C(31)-H(31C)	109.5
C(19)-C(18)-H(18)	119.5	H(31B)-C(31)-H(31C)	109.5
C(18)-C(19)-C(20)	118.4(5)	C(37)-C(32)-C(33)	117.0(3)
C(18)-C(19)-H(19)	120.8	C(37)-C(32)-Pt	119.3(3)
C(20)-C(19)-H(19)	120.8	C(33)-C(32)-Pt	123.4(3)
N(2)-C(20)-C(19)	122.4(4)	C(34)-C(33)-C(32)	121.0(3)
N(2)-C(20)-H(20)	118.8	C(34)-C(33)-C(38)	117.3(3)
C(19)-C(20)-H(20)	118.8	C(32)-C(33)-C(38)	121.7(3)
C(26)-C(21)-C(22)	115.9(4)	C(35)-C(34)-C(33)	120.7(4)
C(26)-C(21)-Pt	124.9(3)	C(35)-C(34)-H(34)	119.6
C(22)-C(21)-Pt	119.1(3)	C(33)-C(34)-H(34)	119.6
C(23)-C(22)-C(21)	121.4(3)	C(34)-C(35)-C(36)	119.6(4)
C(23)-C(22)-C(27)	117.1(3)	C(34)-C(35)-N(4)	122.7(3)
C(21)-C(22)-C(27)	121.5(4)	C(36)-C(35)-N(4)	117.7(3)
C(24)-C(23)-C(22)	120.6(4)	C(35)-C(36)-C(37)	120.3(4)
C(24)-C(23)-H(23)	119.7	C(35)-C(36)-H(36)	119.9
C(22)-C(23)-H(23)	119.7	C(37)-C(36)-H(36)	119.9
C(25)-C(24)-C(23)	120.2(4)	C(36)-C(37)-C(32)	121.4(3)
C(25)-C(24)-N(3)	121.7(3)	C(36)-C(37)-C(39)	116.0(3)
C(23)-C(24)-N(3)	118.1(3)	C(32)-C(37)-C(39)	122.5(3)
C(24)-C(25)-C(26)	120.5(4)	C(33)-C(38)-H(38A)	109.5
C(24)-C(25)-H(25)	119.7	C(33)-C(38)-H(38B)	109.5
C(26)-C(25)-H(25)	119.7	H(38A)-C(38)-H(38B)	109.5
C(25)-C(26)-C(21)	121.4(4)	C(33)-C(38)-H(38C)	109.5
C(25)-C(26)-C(28)	117.1(3)	H(38A)-C(38)-H(38C)	109.5
C(21)-C(26)-C(28)	121.5(4)	H(38B)-C(38)-H(38C)	109.5
C(22)-C(27)-H(27A)	109.5	C(37)-C(39)-H(39A)	109.5
C(22)-C(27)-H(27B)	109.5	C(37)-C(39)-H(39B)	109.5
H(27A)-C(27)-H(27B)	109.5	H(39A)-C(39)-H(39B)	109.5
C(22)-C(27)-H(27C)	109.5	C(37)-C(39)-H(39C)	109.5
H(27A)-C(27)-H(27C)	109.5	H(39A)-C(39)-H(39C)	109.5
H(27B)-C(27)-H(27C)	109.5	H(39B)-C(39)-H(39C)	109.5
C(26)-C(28)-H(28A)	109.5	N(4)-C(40)-H(40A)	109.5
C(26)-C(28)-H(28B)	109.5	N(4)-C(40)-H(40B)	109.5
H(28A)-C(28)-H(28B)	109.5	H(40A)-C(40)-H(40B)	109.5
C(26)-C(28)-H(28C)	109.5	N(4)-C(40)-H(40C)	109.5
H(28A)-C(28)-H(28C)	109.5	H(40A)-C(40)-H(40C)	109.5
H(28B)-C(28)-H(28C)	109.5	H(40B)-C(40)-H(40C)	109.5
N(3)-C(29)-H(29A)	109.5	N(4)-C(41)-H(41A)	109.5
N(3)-C(29)-H(29B)	109.5	N(4)-C(41)-H(41B)	109.5
H(29A)-C(29)-H(29B)	109.5	H(41A)-C(41)-H(41B)	109.5
N(3)-C(29)-H(29C)	109.5	N(4)-C(41)-H(41C)	109.5
H(29A)-C(29)-H(29C)	109.5	H(41A)-C(41)-H(41C)	109.5
H(29B)-C(29)-H(29C)	109.5	H(41B)-C(41)-H(41C)	109.5
N(3)-C(30)-H(30A)	109.5	N(4)-C(42)-H(42A)	109.5
N(3)-C(30)-H(30B)	109.5	N(4)-C(42)-H(42B)	109.5
H(30A)-C(30)-H(30B)	109.5	H(42A)-C(42)-H(42B)	109.5
N(3)-C(30)-H(30C)	109.5	N(4)-C(42)-H(42C)	109.5
H(30A)-C(30)-H(30C)	109.5	H(42A)-C(42)-H(42C)	109.5
H(30B)-C(30)-H(30C)	109.5	H(42B)-C(42)-H(42C)	109.5

C(61)-N(61)-C(62)	121.4(4)	H(72A)-C(72)-H(72C)	109.5
C(61)-N(61)-C(63)	121.7(4)	H(72B)-C(72)-H(72C)	109.5
C(62)-N(61)-C(63)	116.8(4)	N(71)-C(73)-H(73A)	109.5
O(61)-C(61)-N(61)	125.5(5)	N(71)-C(73)-H(73B)	109.5
O(61)-C(61)-H(61)	117.3	H(73A)-C(73)-H(73B)	109.5
N(61)-C(61)-H(61)	117.3	N(71)-C(73)-H(73C)	109.5
N(61)-C(62)-H(62A)	109.5	H(73A)-C(73)-H(73C)	109.5
N(61)-C(62)-H(62B)	109.5	H(73B)-C(73)-H(73C)	109.5
H(62A)-C(62)-H(62B)	109.5	C(81)-N(81)-C(83)	122.5(3)
N(61)-C(62)-H(62C)	109.5	C(81)-N(81)-C(82)	120.3(3)
H(62A)-C(62)-H(62C)	109.5	C(83)-N(81)-C(82)	117.2(3)
H(62B)-C(62)-H(62C)	109.5	O(81)-C(81)-N(81)	126.0(4)
N(61)-C(63)-H(63A)	109.5	O(81)-C(81)-H(81)	117.0
N(61)-C(63)-H(63B)	109.5	N(81)-C(81)-H(81)	117.0
H(63A)-C(63)-H(63B)	109.5	N(81)-C(82)-H(82A)	109.5
N(61)-C(63)-H(63C)	109.5	N(81)-C(82)-H(82B)	109.5
H(63A)-C(63)-H(63C)	109.5	H(82A)-C(82)-H(82B)	109.5
H(63B)-C(63)-H(63C)	109.5	N(81)-C(82)-H(82C)	109.5
C(71)-N(71)-C(73)	121.2(4)	H(82A)-C(82)-H(82C)	109.5
C(71)-N(71)-C(72)	123.4(4)	H(82B)-C(82)-H(82C)	109.5
C(73)-N(71)-C(72)	115.4(4)	N(81)-C(83)-H(83A)	109.5
O(71)-C(71)-N(71)	124.8(5)	N(81)-C(83)-H(83B)	109.5
O(71)-C(71)-H(71)	117.6	H(83A)-C(83)-H(83B)	109.5
N(71)-C(71)-H(71)	117.6	N(81)-C(83)-H(83C)	109.5
N(71)-C(72)-H(72A)	109.5	H(83A)-C(83)-H(83C)	109.5
N(71)-C(72)-H(72B)	109.5	H(83B)-C(83)-H(83C)	109.5
H(72A)-C(72)-H(72B)	109.5	H(91A)-O(91)-H(91B)	120.4
N(71)-C(72)-H(72C)	109.5	H(92A)-O(92)-H(92B)	111.3

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for DAV12 (CCDC 161166). 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}
Pt	174(1)	284(1)	194(1)	73(1)	57(1)	119(1)
Cl(1)	597(9)	311(7)	632(8)	179(6)	348(7)	226(7)
Cl(2)	356(8)	1320(15)	380(7)	-33(9)	22(6)	273(9)
N(1)	230(20)	370(20)	240(19)	175(18)	138(16)	179(19)
N(2)	183(19)	340(20)	256(19)	72(18)	77(16)	119(18)
N(3)	234(19)	210(20)	310(20)	56(16)	53(16)	106(17)
N(4)	209(19)	210(20)	310(20)	40(16)	36(16)	81(16)
C(1)	250(20)	510(30)	210(20)	140(20)	139(19)	240(20)
C(2)	180(20)	510(30)	170(20)	70(20)	58(18)	170(20)
C(3)	270(30)	400(30)	350(30)	170(20)	170(20)	190(20)
C(4)	420(30)	490(30)	500(30)	310(30)	270(30)	320(30)
C(5)	420(30)	630(40)	430(30)	350(30)	300(30)	400(30)
C(6)	280(30)	680(40)	220(20)	200(20)	160(20)	300(30)
C(7)	360(30)	790(40)	260(30)	200(30)	200(20)	400(30)
C(8)	390(30)	1080(50)	210(20)	250(30)	170(20)	490(30)
C(9)	430(30)	1200(60)	270(30)	210(30)	190(30)	540(40)
C(10)	470(30)	1470(60)	250(30)	250(30)	130(30)	660(40)
C(11)	650(50)	1690(80)	380(40)	160(50)	240(30)	760(50)
C(12)	360(30)	1400(60)	190(30)	-100(40)	-60(20)	490(40)
C(13)	540(40)	1490(60)	350(30)	-210(40)	20(30)	650(40)
C(14)	300(30)	1310(60)	140(20)	-70(30)	-10(20)	480(40)
C(15)	360(30)	900(40)	320(30)	-90(30)	20(20)	390(30)
C(16)	290(30)	880(40)	170(20)	30(30)	60(20)	360(30)
C(17)	250(30)	550(40)	250(20)	20(20)	80(20)	200(30)
C(18)	160(20)	690(40)	330(30)	-90(30)	-20(20)	130(30)
C(19)	260(30)	430(30)	470(30)	-30(30)	20(20)	60(20)
C(20)	220(20)	460(30)	320(30)	20(20)	20(20)	140(20)
C(21)	200(20)	200(20)	240(20)	57(18)	79(18)	140(19)
C(22)	200(20)	250(20)	190(20)	62(18)	49(17)	130(20)
C(23)	220(20)	260(30)	260(20)	82(19)	102(19)	140(20)
C(24)	200(20)	210(20)	250(20)	41(19)	38(18)	110(20)
C(25)	220(20)	320(30)	240(20)	30(20)	63(19)	180(20)
C(26)	220(20)	270(30)	210(20)	93(19)	114(18)	180(20)
C(27)	250(20)	330(30)	250(20)	50(20)	130(20)	100(20)
C(28)	330(30)	330(30)	190(20)	94(19)	118(19)	150(20)
C(29)	420(30)	250(30)	480(30)	120(20)	10(20)	120(20)
C(30)	350(30)	280(30)	290(20)	-30(20)	0(20)	100(20)
C(31)	250(30)	360(30)	510(30)	10(20)	100(20)	100(20)
C(32)	160(20)	190(20)	170(20)	27(18)	0(17)	35(18)
C(33)	150(20)	220(20)	132(19)	-43(17)	-24(16)	50(18)
C(34)	140(20)	280(30)	220(20)	-33(19)	33(17)	67(19)
C(35)	160(20)	190(20)	250(20)	12(18)	-13(18)	102(19)
C(36)	170(20)	230(20)	220(20)	54(19)	34(18)	31(19)
C(37)	150(20)	220(20)	200(20)	24(18)	28(17)	61(18)
C(38)	230(20)	280(30)	220(20)	15(19)	60(18)	110(20)
C(39)	220(20)	290(30)	280(20)	70(20)	93(19)	110(20)
C(40)	310(30)	280(30)	330(30)	70(20)	-30(20)	140(20)

C(41)	270(30)	280(30)	510(30)	100(20)	110(20)	170(20)
C(42)	220(20)	200(30)	490(30)	50(20)	70(20)	40(20)
N(61)	310(20)	380(30)	340(20)	100(20)	53(18)	160(20)
O(61)	1450(40)	820(30)	480(20)	60(20)	110(20)	920(30)
C(61)	480(30)	620(40)	410(30)	150(30)	90(30)	370(30)
C(62)	430(30)	460(30)	350(30)	90(20)	90(20)	240(30)
C(63)	610(40)	400(40)	440(30)	50(30)	-60(30)	100(30)
N(71)	360(20)	300(20)	550(30)	-40(20)	0(20)	120(20)
O(71)	710(30)	740(30)	660(30)	-50(20)	-250(20)	300(20)
C(71)	510(40)	370(30)	540(40)	10(30)	-40(30)	120(30)
C(72)	390(30)	440(40)	930(40)	-240(30)	20(30)	180(30)
C(73)	420(30)	360(30)	430(30)	-30(20)	10(20)	150(30)
N(81)	190(18)	210(20)	255(18)	36(16)	76(15)	87(16)
O(81)	291(17)	241(18)	381(17)	70(15)	59(14)	118(15)
C(81)	170(20)	290(30)	260(20)	-20(20)	10(18)	60(20)
C(82)	250(20)	300(30)	260(20)	-10(20)	60(20)	90(20)
C(83)	270(20)	270(30)	320(20)	40(20)	70(20)	130(20)
O(91)	860(30)	1860(50)	690(30)	-70(30)	50(20)	1000(40)
O(92)	860(40)	940(40)	1640(50)	250(40)	0(30)	240(30)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for DAV12 (CCDC 161166).

	x	y	z	U_{iso}
H(3)	9562	11613	6916	37
H(4)	8482	12414	6000	47
H(5)	6778	11562	4765	47
H(8)	5322	10730	3664	58
H(10)	3566	10604	2343	77
H(11)	1832	9695	1220	96
H(12)	1057	8028	1068	77
H(13)	2126	7208	2058	90
H(15)	3898	7341	3408	60
H(18)	4835	6729	4386	51
H(19)	6022	6105	5462	52
H(20)	7832	7178	6548	41
H(23)	13130	12346	7032	27
H(25)	12772	11966	9581	29
H(27A)	10481	11039	5713	41
H(27B)	11029	10225	5821	41
H(27C)	11869	11306	5732	41
H(28A)	11331	10619	9863	40
H(28B)	10530	9702	9080	40
H(28C)	10048	10537	9174	40
H(29A)	13404	14128	8483	62
H(29B)	13857	13897	7641	62
H(29C)	14826	14607	8554	62
H(30A)	15358	14014	9990	50
H(30B)	14729	12891	10083	50
H(30C)	13945	13543	9947	50
H(31A)	15131	12940	7855	57
H(31B)	15426	12508	8812	57
H(31C)	16051	13646	8786	57
H(34)	11809	7350	7551	27
H(36)	9355	6831	8982	27
H(38A)	12215	8571	6691	37
H(38B)	11862	9462	6873	37
H(38C)	10960	8597	6057	37
H(39A)	7589	7582	8030	38
H(39B)	8419	8707	8363	38
H(39C)	8431	7944	9087	38
H(40A)	12181	7019	9909	49
H(40B)	11685	5895	10023	49
H(40C)	10847	6485	10026	49
H(41A)	11491	5770	7682	50
H(41B)	11987	5415	8645	50
H(41C)	12591	6527	8507	50
H(42A)	9210	5325	8804	48
H(42B)	9992	4707	8714	48
H(42C)	9391	5112	7822	48
H(61)	3386	6840	5730	56
H(62A)	4912	7168	8048	60

H(62B)	5498	6408	7923	60
H(62C)	4193	6048	8105	60
H(63A)	3270	4901	6542	84
H(63B)	4621	5297	6440	84
H(63C)	3527	5404	5652	84
H(71)	9958	5838	3559	64
H(72A)	8121	6709	4359	94
H(72B)	9216	7279	5280	94
H(72C)	8303	6192	5274	94
H(73A)	10947	5907	5061	64
H(73B)	10178	5822	5778	64
H(73C)	11086	6861	5645	64
H(81)	4671	8832	8492	31
H(82A)	2210	9039	9337	41
H(82B)	3290	9959	10013	41
H(82C)	3259	8899	10144	41
H(83A)	4451	10206	8115	42
H(83B)	4532	10842	9011	42
H(83C)	3242	10287	8234	42
H(91A)	7008	4964	6935	50
H(91B)	6653	5199	7905	50
H(92A)	8849	6332	886	50
H(92B)	9154	6489	1900	50

Table 7. Hydrogen bonds for DAV12 (CCDC 161166) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(91)-H(91B)...Cl(1)	0.89	2.42	3.294(4)	164.2
O(91)-H(91A)...Cl(2)	1.07	2.08	3.145(4)	174.9
O(92)-H(92A)...Cl(1)#1	0.88	2.20	3.084(5)	178.2
O(92)-H(92B)...O(71)	0.89	2.02	2.907(7)	178.0

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