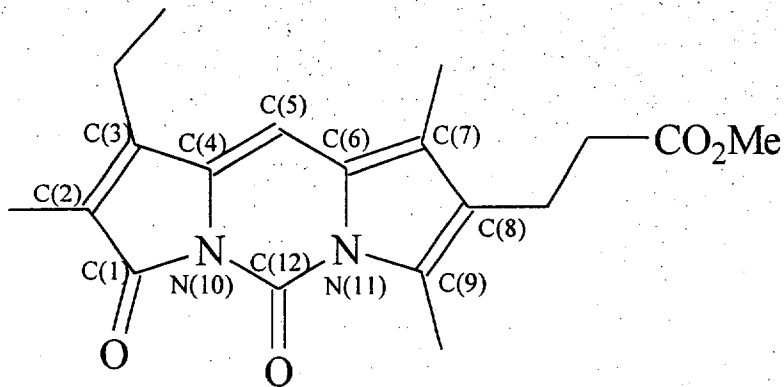


Supporting Information for

# SUPPORTING INFORMATION

## Synthesis and Spectroscopic Properties of New Class of Strongly Fluorescent Dipyrinones

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Table 1. Crystal data and structure refinement for vjc280.

Identification code	vjc280	
Empirical formula	C <sub>20</sub> H <sub>24</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>4</sub>	
Formula weight	427.31	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.1880(10) Å	α = 85.040(10)°
	b = 10.232(2) Å	β = 68.170(10)°
	c = 12.188(2) Å	γ = 81.210(10)°
Volume	1050.6(3) Å <sup>3</sup>	
Z	2	
Density (calculated)	1.351 Mg/m <sup>3</sup>	
Absorption coefficient	0.337 mm <sup>-1</sup>	
F(000)	448	
Crystal size	.12 x .38 x .12 mm <sup>3</sup>	
Theta range for data collection	2.41 to 22.50°	
Index ranges	-9 ≤ h ≤ 1, -11 ≤ k ≤ 10, -13 ≤ l ≤ 12	
Reflections collected	3348	
Independent reflections	2733 [R(int) = 0.0582]	
Completeness to theta = 22.50°	99.9 %	
Absorption correction	Empirical	
Max. and min. transmission	0.6969 and 0.6772	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	2733 / 0 / 254	
Goodness-of-fit on F <sup>2</sup>	1.019	
Final R indices [I > 2σ(I)]	R1 = 0.0754, wR2 = 0.1040	
R indices (all data)	R1 = 0.1888, wR2 = 0.1338	
Extinction coefficient	0.0054(12)	
Largest diff. peak and hole	0.210 and -0.193 e.Å <sup>-3</sup>	

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for vjc280.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{\text{ij}}$  tensor.

	x	y	z	$U(\text{eq})$
O(1)	3788(6)	8532(4)	4314(4)	75(2)
O(12)	2698(5)	6849(4)	3155(4)	67(2)
O(83)	-227(6)	597(5)	1926(4)	82(2)
O(84)	2194(6)	-483(5)	1200(4)	76(2)
N(10)	3110(6)	6401(5)	4900(4)	44(1)
N(11)	2182(6)	4849(5)	4133(4)	43(1)
C(1)	3602(8)	7621(7)	5029(6)	54(2)
C(2)	3869(7)	7484(6)	6144(6)	50(2)
C(3)	3564(7)	6287(6)	6637(6)	48(2)
C(4)	3073(7)	5557(6)	5892(5)	42(2)
C(5)	2602(7)	4356(6)	5992(5)	43(2)
C(6)	2124(7)	3960(6)	5097(5)	43(2)
C(7)	1552(7)	2855(6)	4942(5)	45(2)
C(8)	1238(7)	3061(6)	3885(6)	47(2)
C(9)	1628(7)	4271(7)	3392(5)	49(2)
C(12)	2657(7)	6106(7)	3985(6)	46(2)
C(21)	4347(8)	8600(6)	6604(5)	75(2)
C(31)	3623(8)	5742(6)	7800(6)	63(2)
C(32)	1986(8)	5887(6)	8791(5)	78(2)
C(71)	1271(8)	1670(5)	5777(5)	68(2)
C(81)	562(7)	2116(6)	3386(5)	61(2)
C(82)	1795(7)	1110(6)	2577(5)	57(2)
C(83)	1104(10)	402(7)	1880(6)	54(2)
C(84)	1675(9)	-1261(6)	505(6)	103(3)
C(91)	1554(7)	4933(6)	2257(5)	62(2)
C(1S)	4425(8)	1742(7)	8783(6)	88(3)
Cl(1S)	2612(3)	1885(3)	8652(2)	134(1)
Cl(2S)	4472(3)	2881(2)	9772(2)	121(1)

Table 3. Bond lengths [Å] and angles [°] for vjc280.

O(1)-C(1)	1.206(6)	C(9)-N(11)-C(6)	108.1(5)
O(12)-C(12)	1.204(6)	O(1)-C(1)-N(10)	124.8(7)
O(83)-C(83)	1.189(7)	O(1)-C(1)-C(2)	129.2(7)
O(84)-C(83)	1.320(7)	N(10)-C(1)-C(2)	106.0(5)
O(84)-C(84)	1.453(6)	C(3)-C(2)-C(1)	109.1(6)
N(10)-C(12)	1.397(7)	C(3)-C(2)-C(21)	129.4(7)
N(10)-C(4)	1.416(7)	C(1)-C(2)-C(21)	121.4(6)
N(10)-C(1)	1.430(7)	C(2)-C(3)-C(4)	109.9(6)
N(11)-C(12)	1.396(7)	C(2)-C(3)-C(31)	127.5(6)
N(11)-C(9)	1.397(7)	C(4)-C(3)-C(31)	122.5(6)
N(11)-C(6)	1.412(6)	C(5)-C(4)-N(10)	120.1(6)
C(1)-C(2)	1.461(8)	C(5)-C(4)-C(3)	133.7(6)
C(2)-C(3)	1.339(7)	N(10)-C(4)-C(3)	106.2(5)
C(2)-C(21)	1.502(7)	C(4)-C(5)-C(6)	119.0(6)
C(3)-C(4)	1.454(7)	C(7)-C(6)-N(11)	107.8(5)
C(3)-C(31)	1.494(7)	C(7)-C(6)-C(5)	134.1(6)
C(4)-C(5)	1.345(7)	N(11)-C(6)-C(5)	118.1(6)
C(5)-C(6)	1.426(7)	C(6)-C(7)-C(8)	107.5(5)
C(6)-C(7)	1.372(7)	C(6)-C(7)-C(71)	125.4(6)
C(7)-C(8)	1.414(7)	C(8)-C(7)-C(71)	127.0(6)
C(7)-C(71)	1.503(7)	C(9)-C(8)-C(7)	109.1(6)
C(8)-C(9)	1.367(7)	C(9)-C(8)-C(81)	125.2(6)
C(8)-C(81)	1.502(7)	C(7)-C(8)-C(81)	125.7(6)
C(9)-C(91)	1.508(7)	C(8)-C(9)-N(11)	107.5(6)
C(31)-C(32)	1.535(8)	C(8)-C(9)-C(91)	129.7(6)
C(81)-C(82)	1.518(7)	N(11)-C(9)-C(91)	122.8(6)
C(82)-C(83)	1.516(8)	O(12)-C(12)-N(11)	124.2(6)
C(1S)-Cl(1S)	1.715(7)	O(12)-C(12)-N(10)	123.5(6)
C(1S)-Cl(2S)	1.764(6)	N(11)-C(12)-N(10)	112.3(6)
		C(3)-C(31)-C(32)	112.3(5)
C(83)-O(84)-C(84)	116.1(5)	C(8)-C(81)-C(82)	114.1(5)
C(12)-N(10)-C(4)	125.1(6)	C(83)-C(82)-C(81)	111.7(5)
C(12)-N(10)-C(1)	126.1(6)	O(83)-C(83)-O(84)	123.8(7)
C(4)-N(10)-C(1)	108.7(5)	O(83)-C(83)-C(82)	125.8(7)
C(12)-N(11)-C(9)	126.6(6)	O(84)-C(83)-C(82)	110.4(6)
C(12)-N(11)-C(6)	125.3(5)	Cl(1S)-C(1S)-Cl(2S)	112.1(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for vjc280. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
O(1)	106(4)	53(3)	70(4)	11(3)	-27(3)	-39(3)
O(12)	92(4)	61(3)	52(3)	16(3)	-29(3)	-24(3)
O(83)	56(4)	99(4)	97(4)	-33(3)	-31(4)	-7(3)
O(84)	73(4)	72(3)	99(4)	-42(3)	-50(3)	15(3)
N(10)	44(4)	39(3)	48(4)	1(3)	-13(3)	-15(3)
N(11)	52(4)	38(3)	40(3)	-1(3)	-16(3)	-11(3)
C(1)	59(5)	48(5)	49(5)	2(4)	-11(4)	-11(4)
C(2)	45(5)	44(4)	57(5)	-4(4)	-14(4)	-7(4)
C(3)	46(5)	56(5)	48(5)	-6(4)	-23(4)	-2(4)
C(4)	41(5)	36(4)	44(4)	3(4)	-12(4)	-4(4)
C(5)	41(4)	40(4)	39(4)	3(3)	-5(4)	-2(4)
C(6)	46(5)	43(5)	42(4)	-9(4)	-20(4)	4(4)
C(7)	57(5)	39(4)	42(4)	-9(3)	-18(4)	-8(4)
C(8)	42(5)	37(4)	55(5)	-13(4)	-7(4)	-4(4)
C(9)	46(5)	57(5)	44(5)	-13(4)	-20(4)	4(4)
C(12)	38(5)	49(5)	43(5)	-12(4)	-3(4)	-4(4)
C(21)	80(6)	60(5)	87(5)	-15(4)	-25(5)	-25(5)
C(31)	71(6)	63(5)	60(5)	-9(4)	-27(5)	-13(4)
C(32)	91(7)	96(6)	45(5)	-8(4)	-25(5)	-5(5)
C(71)	79(6)	39(4)	86(5)	4(4)	-28(5)	-19(4)
C(81)	62(6)	58(5)	67(5)	-7(4)	-25(5)	-15(4)
C(82)	56(5)	61(5)	63(5)	-18(4)	-27(4)	-14(4)
C(83)	59(6)	50(5)	52(5)	2(4)	-22(5)	-2(5)
C(84)	126(8)	86(6)	121(7)	-61(5)	-65(6)	-2(6)
C(91)	70(6)	67(5)	51(5)	-7(4)	-24(4)	-11(4)
C(1S)	87(7)	92(6)	82(6)	-5(5)	-29(5)	-6(5)
Cl(1S)	98(2)	157(3)	158(2)	50(2)	-64(2)	-41(2)
Cl(2S)	121(2)	146(2)	86(2)	-17(2)	-31(2)	-3(2)

Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for vjc280.

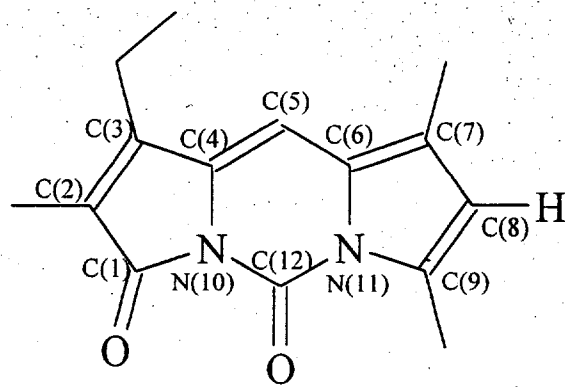
	x	y	z	U(eq)
H(5A)	2589	3792	6635	52
H(21A)	4465	8328	7343	112
H(21B)	3548	9353	6719	112
H(21C)	5333	8831	6043	112
H(31A)	4328	6200	8009	76
H(31B)	4052	4813	7725	76
H(32A)	2079	5525	9520	116
H(32B)	1290	5419	8596	116
H(32C)	1566	6806	8879	116
H(71A)	1586	1792	6425	102
H(71B)	1880	892	5366	102
H(71C)	168	1568	6073	102
H(81A)	-40	2619	2949	73
H(81B)	-164	1647	4036	73
H(82A)	2655	1556	2032	68
H(82B)	2224	466	3046	68
H(84A)	2551	-1869	44	154
H(84B)	1279	-683	-13	154
H(84C)	853	-1745	1024	154
H(91A)	1143	4371	1882	93
H(91B)	2596	5089	1738	93
H(91C)	875	5760	2426	93
H(1SA)	5224	1887	8012	105
H(1SB)	4680	850	9060	105

Table 6. Torsion angles [°] for vjc280.

C(12)-N(10)-C(1)-O(1)	-5.1(11)	C(5)-C(6)-C(7)-C(71)	-0.1(12)
C(4)-N(10)-C(1)-O(1)	178.0(7)	C(6)-C(7)-C(8)-C(9)	0.7(7)
C(12)-N(10)-C(1)-C(2)	177.0(5)	C(71)-C(7)-C(8)-C(9)	178.8(6)
C(4)-N(10)-C(1)-C(2)	0.2(7)	C(6)-C(7)-C(8)-C(81)	-178.6(6)
O(1)-C(1)-C(2)-C(3)	-177.7(7)	C(71)-C(7)-C(8)-C(81)	-0.4(10)
N(10)-C(1)-C(2)-C(3)	0.0(8)	C(7)-C(8)-C(9)-N(11)	-0.4(7)
O(1)-C(1)-C(2)-C(21)	4.5(12)	C(81)-C(8)-C(9)-N(11)	178.8(5)
N(10)-C(1)-C(2)-C(21)	-177.7(5)	C(7)-C(8)-C(9)-C(91)	178.3(6)
C(1)-C(2)-C(3)-C(4)	-0.2(8)	C(81)-C(8)-C(9)-C(91)	-2.5(11)
C(21)-C(2)-C(3)-C(4)	177.3(6)	C(12)-N(11)-C(9)-C(8)	-177.7(5)
C(1)-C(2)-C(3)-C(31)	-177.6(6)	C(6)-N(11)-C(9)-C(8)	0.0(7)
C(21)-C(2)-C(3)-C(31)	0.0(12)	C(12)-N(11)-C(9)-C(91)	3.5(9)
C(12)-N(10)-C(4)-C(5)	1.3(9)	C(6)-N(11)-C(9)-C(91)	-178.8(5)
C(1)-N(10)-C(4)-C(5)	178.2(6)	C(9)-N(11)-C(12)-O(12)	-2.7(10)
C(12)-N(10)-C(4)-C(3)	-177.2(5)	C(6)-N(11)-C(12)-O(12)	-180.0(6)
C(1)-N(10)-C(4)-C(3)	-0.3(6)	C(9)-N(11)-C(12)-N(10)	178.4(5)
C(2)-C(3)-C(4)-C(5)	-177.9(7)	C(6)-N(11)-C(12)-N(10)	1.1(8)
C(31)-C(3)-C(4)-C(5)	-0.4(11)	C(4)-N(10)-C(12)-O(12)	179.8(6)
C(2)-C(3)-C(4)-N(10)	0.3(7)	C(1)-N(10)-C(12)-O(12)	3.4(10)
C(31)-C(3)-C(4)-N(10)	177.8(6)	C(4)-N(10)-C(12)-N(11)	-1.3(8)
N(10)-C(4)-C(5)-C(6)	-0.9(9)	C(1)-N(10)-C(12)-N(11)	-177.7(5)
C(3)-C(4)-C(5)-C(6)	177.1(6)	C(2)-C(3)-C(31)-C(32)	97.0(8)
C(12)-N(11)-C(6)-C(7)	178.1(5)	C(4)-C(3)-C(31)-C(32)	-80.1(7)
C(9)-N(11)-C(6)-C(7)	0.4(7)	C(9)-C(8)-C(81)-C(82)	92.4(8)
C(12)-N(11)-C(6)-C(5)	-0.8(9)	C(7)-C(8)-C(81)-C(82)	-88.5(8)
C(9)-N(11)-C(6)-C(5)	-178.5(5)	C(8)-C(81)-C(82)-C(83)	-166.6(5)
C(4)-C(5)-C(6)-C(7)	-177.9(7)	C(84)-O(84)-C(83)-O(83)	-1.5(10)
C(4)-C(5)-C(6)-N(11)	0.7(9)	C(84)-O(84)-C(83)-C(82)	178.4(5)
N(11)-C(6)-C(7)-C(8)	-0.6(7)	C(81)-C(82)-C(83)-O(83)	1.0(10)
C(5)-C(6)-C(7)-C(8)	178.0(6)	C(81)-C(82)-C(83)-O(84)	-178.9(5)
N(11)-C(6)-C(7)-C(71)	-178.8(6)		

Symmetry transformations used to generate equivalent atoms:





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Table 1. Crystal data and structure refinement for vjc290.

Identification code	vjc290	
Empirical formula	C <sub>16</sub> H <sub>18</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	
Formula weight	341.22	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 8.2590(10) Å	α = 90°.
	b = 15.3980(10) Å	β = 93.740(10)°.
	c = 13.044(2) Å	γ = 90°.
Volume	1655.3(3) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.369 Mg/m <sup>3</sup>	
Absorption coefficient	0.400 mm <sup>-1</sup>	
F(000)	712	
Crystal size	.42 x .22 x .20 mm <sup>3</sup>	
Theta range for data collection	2.65 to 25.00°.	
Index ranges	-1 ≤ h ≤ 9, -1 ≤ k ≤ 18, -15 ≤ l ≤ 15	
Reflections collected	3846	
Independent reflections	2914 [R(int) = 0.0463]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	2914 / 0 / 203	
Goodness-of-fit on F <sup>2</sup>	1.005	
Final R indices [I > 2σ(I)]	R1 = 0.0757, wR2 = 0.1282	
R indices (all data)	R1 = 0.1988, wR2 = 0.1683	
Largest diff. peak and hole	0.327 and -0.235 e.Å <sup>-3</sup>	

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for vjc290.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{\text{ij}}$  tensor.

	x	y	z	U(eq)
O(1)	4599(5)	7083(2)	3347(3)	64(1)
O(12)	2921(5)	6861(2)	5160(3)	62(1)
N(10)	3606(5)	5797(2)	4039(3)	40(1)
N(11)	2209(5)	5447(2)	5465(3)	42(1)
C(1)	4398(7)	6309(3)	3303(4)	47(1)
C(2)	4921(7)	5691(3)	2534(3)	46(1)
C(21)	5762(7)	5993(4)	1618(4)	67(2)
C(3)	4500(6)	4873(3)	2793(4)	42(1)
C(31)	4713(7)	4052(3)	2221(4)	51(2)
C(32)	3282(8)	3855(4)	1475(4)	84(2)
C(4)	3671(6)	4913(3)	3742(4)	39(1)
C(5)	3050(6)	4303(3)	4338(3)	41(1)
C(6)	2268(6)	4552(3)	5229(4)	39(1)
C(7)	1469(7)	4116(4)	5962(4)	50(2)
C(71)	1236(7)	3149(3)	6008(4)	65(2)
C(8)	891(7)	4744(3)	6628(4)	52(2)
C(9)	1327(6)	5555(3)	6339(4)	46(1)
C(91)	939(7)	6416(3)	6785(4)	64(2)
C(12)	2920(7)	6109(3)	4912(4)	46(1)
C(1S)	4714(8)	1494(4)	4713(4)	76(2)
Cl(1S)	3723(3)	1855(1)	3567(1)	95(1)
Cl(2S)	3450(3)	843(1)	5410(1)	99(1)

Table 3. Bond lengths [Å] and angles [°] for vjc290.

O(1)-C(1)	1.203(5)	C(9)-N(11)-C(6)	108.7(4)
O(12)-C(12)	1.201(5)	O(1)-C(1)-N(10)	125.5(5)
N(10)-C(12)	1.391(6)	O(1)-C(1)-C(2)	128.9(5)
N(10)-C(4)	1.417(5)	N(10)-C(1)-C(2)	105.6(4)
N(10)-C(1)	1.432(6)	C(3)-C(2)-C(1)	109.9(4)
N(11)-C(12)	1.400(6)	C(3)-C(2)-C(21)	128.9(5)
N(11)-C(9)	1.401(6)	C(1)-C(2)-C(21)	121.1(5)
N(11)-C(6)	1.413(6)	C(2)-C(3)-C(4)	108.4(4)
C(1)-C(2)	1.468(7)	C(2)-C(3)-C(31)	128.8(5)
C(2)-C(3)	1.355(6)	C(4)-C(3)-C(31)	122.8(4)
C(2)-C(21)	1.496(6)	C(3)-C(31)-C(32)	112.4(5)
C(3)-C(4)	1.455(6)	C(5)-C(4)-N(10)	119.5(4)
C(3)-C(31)	1.485(6)	C(5)-C(4)-C(3)	133.0(5)
C(31)-C(32)	1.512(7)	N(10)-C(4)-C(3)	107.5(4)
C(4)-C(5)	1.342(6)	C(4)-C(5)-C(6)	119.8(4)
C(5)-C(6)	1.419(6)	C(7)-C(6)-N(11)	107.5(4)
C(6)-C(7)	1.371(6)	C(7)-C(6)-C(5)	134.7(5)
C(7)-C(8)	1.404(7)	N(11)-C(6)-C(5)	117.8(4)
C(7)-C(71)	1.504(7)	C(6)-C(7)-C(8)	107.0(5)
C(8)-C(9)	1.360(7)	C(6)-C(7)-C(71)	125.6(5)
C(9)-C(91)	1.491(6)	C(8)-C(7)-C(71)	127.4(5)
C(1S)-Cl(2S)	1.745(6)	C(9)-C(8)-C(7)	110.7(5)
C(1S)-Cl(1S)	1.747(6)	C(8)-C(9)-N(11)	106.1(4)
		C(8)-C(9)-C(91)	129.9(5)
C(12)-N(10)-C(4)	125.5(4)	N(11)-C(9)-C(91)	124.0(5)
C(12)-N(10)-C(1)	125.9(4)	O(12)-C(12)-N(10)	124.1(5)
C(4)-N(10)-C(1)	108.6(4)	O(12)-C(12)-N(11)	123.7(5)
C(12)-N(11)-C(9)	126.2(4)	N(10)-C(12)-N(11)	112.2(4)
C(12)-N(11)-C(6)	125.2(4)	Cl(2S)-C(1S)-Cl(1S)	111.4(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for vjc290. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [h^2 a^* U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
O(1)	80(3)	43(2)	69(3)	1(2)	15(2)	-11(2)
O(12)	75(3)	41(2)	73(3)	-11(2)	21(2)	-5(2)
N(10)	45(3)	34(2)	43(2)	0(2)	7(2)	-3(2)
N(11)	41(3)	42(3)	43(2)	-1(2)	7(2)	0(2)
C(1)	46(4)	49(3)	44(3)	4(3)	-6(3)	-5(3)
C(2)	47(4)	52(3)	38(3)	3(3)	4(3)	4(3)
C(21)	76(5)	70(4)	59(4)	6(3)	23(4)	-3(4)
C(3)	40(4)	44(3)	42(3)	-4(3)	4(3)	0(3)
C(31)	51(4)	52(3)	52(3)	-5(3)	14(3)	4(3)
C(32)	91(6)	75(4)	83(5)	-28(4)	-11(4)	9(4)
C(4)	37(4)	35(3)	45(3)	-2(3)	-5(3)	-1(3)
C(5)	41(4)	34(3)	48(3)	-3(3)	-2(3)	8(3)
C(6)	35(3)	37(3)	46(3)	-1(3)	-1(3)	2(3)
C(7)	47(4)	53(3)	51(3)	7(3)	4(3)	-2(3)
C(71)	70(5)	57(4)	69(4)	11(3)	16(4)	-13(4)
C(8)	45(4)	67(4)	44(3)	9(3)	12(3)	2(3)
C(9)	33(4)	57(4)	49(3)	2(3)	1(3)	9(3)
C(91)	62(4)	72(4)	59(3)	-5(3)	13(3)	14(4)
C(12)	37(4)	49(4)	50(3)	1(3)	-4(3)	3(3)
C(1S)	87(5)	66(4)	76(4)	3(3)	8(4)	-12(4)
Cl(1S)	128(2)	83(1)	72(1)	1(1)	-3(1)	-12(1)
Cl(2S)	124(2)	89(1)	88(1)	4(1)	31(1)	-24(1)

Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for vjc290.

	x	y	z	U(eq)
H(21A)	6282	5509	1313	101
H(21B)	6561	6422	1827	101
H(21C)	4982	6244	1125	101
H(31A)	4859	3577	2707	62
H(31B)	5687	4093	1846	62
H(32A)	3489	3330	1107	126
H(32B)	3124	4326	997	126
H(32C)	2325	3782	1846	126
H(5A)	3132	3719	4167	49
H(71A)	1564	2890	5385	98
H(71B)	113	3022	6087	98
H(71C)	1883	2917	6583	98
H(8A)	292	4622	7190	62
H(91A)	302	6333	7367	96
H(91B)	338	6759	6276	96
H(91C)	1929	6711	6999	96
H(1SA)	5670	1165	4559	92
H(1SB)	5066	1991	5126	92

Table 6. Torsion angles [°] for vjc290.

C(12)-N(10)-C(1)-O(1)	1.1(9)	C(9)-N(11)-C(6)-C(7)	-1.4(6)
C(4)-N(10)-C(1)-O(1)	-177.6(6)	C(12)-N(11)-C(6)-C(5)	-2.8(7)
C(12)-N(10)-C(1)-C(2)	179.6(5)	C(9)-N(11)-C(6)-C(5)	177.3(4)
C(4)-N(10)-C(1)-C(2)	1.0(5)	C(4)-C(5)-C(6)-C(7)	176.9(6)
O(1)-C(1)-C(2)-C(3)	177.7(6)	C(4)-C(5)-C(6)-N(11)	-1.4(7)
N(10)-C(1)-C(2)-C(3)	-0.8(6)	N(11)-C(6)-C(7)-C(8)	1.4(6)
O(1)-C(1)-C(2)-C(21)	-3.3(9)	C(5)-C(6)-C(7)-C(8)	-177.0(5)
N(10)-C(1)-C(2)-C(21)	178.2(4)	N(11)-C(6)-C(7)-C(71)	179.9(5)
C(1)-C(2)-C(3)-C(4)	0.3(6)	C(5)-C(6)-C(7)-C(71)	1.5(10)
C(21)-C(2)-C(3)-C(4)	-178.6(5)	C(6)-C(7)-C(8)-C(9)	-0.9(6)
C(1)-C(2)-C(3)-C(31)	176.9(5)	C(71)-C(7)-C(8)-C(9)	-179.4(5)
C(21)-C(2)-C(3)-C(31)	-2.0(10)	C(7)-C(8)-C(9)-N(11)	0.0(6)
C(2)-C(3)-C(31)-C(32)	-89.2(7)	C(7)-C(8)-C(9)-C(91)	177.5(5)
C(4)-C(3)-C(31)-C(32)	86.9(6)	C(12)-N(11)-C(9)-C(8)	-179.0(5)
C(12)-N(10)-C(4)-C(5)	-0.9(8)	C(6)-N(11)-C(9)-C(8)	0.9(6)
C(1)-N(10)-C(4)-C(5)	177.8(4)	C(12)-N(11)-C(9)-C(91)	3.3(8)
C(12)-N(10)-C(4)-C(3)	-179.4(4)	C(6)-N(11)-C(9)-C(91)	-176.8(5)
C(1)-N(10)-C(4)-C(3)	-0.8(5)	C(4)-N(10)-C(12)-O(12)	177.9(5)
C(2)-C(3)-C(4)-C(5)	-178.0(6)	C(1)-N(10)-C(12)-O(12)	-0.5(9)
C(31)-C(3)-C(4)-C(5)	5.2(9)	C(4)-N(10)-C(12)-N(11)	-2.8(7)
C(2)-C(3)-C(4)-N(10)	0.3(6)	C(1)-N(10)-C(12)-N(11)	178.8(4)
C(31)-C(3)-C(4)-N(10)	-176.5(5)	C(9)-N(11)-C(12)-O(12)	3.8(8)
N(10)-C(4)-C(5)-C(6)	3.1(7)	C(6)-N(11)-C(12)-O(12)	-176.1(5)
C(3)-C(4)-C(5)-C(6)	-178.8(5)	C(9)-N(11)-C(12)-N(10)	-175.5(4)
C(12)-N(11)-C(6)-C(7)	178.5(5)	C(6)-N(11)-C(12)-N(10)	4.6(7)

Symmetry transformations used to generate equivalent atoms: