X-Ray crystallographic data tables for paper:

Cycloaddition of Homochiral Dihydroimidazoles: A 1,3-Dipolar Cycloaddition Route to Optically Active Pyrrolo[1,2-*a*]imidazoles

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Crystallographic data tables for compound **9g**

Table 1. Crystal data and structure refinement for **9g**.

Identification code	3js2	
Empirical formula	C27 H34 N2 O4	
Formula weight	450.56	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 8.0460(10) Å	α= 90°.
	b = 14.280(2) Å	β= 90°.
	c = 22.646(3) Å	γ = 90°.
Volume	2602.0(6) $Å^3$	
Z	4	
Density (calculated)	1.150 Mg/m^3	
Absorption coefficient	0.077 mm^{-1}	
F(000)	968	
Crystal size	0.70 x 0.59 x 0.30 mm^3	
Theta range for data collection	2.30 to 25.00°.	
Index ranges	0<=h<=9, 0<=k<=16, 0<=l<=26	
Reflections collected	2631	
Independent reflections	2620 [R(int) = 0.2758]	
Completeness to theta = 25.00°	99.8 %	
Max. and min. transmission	0.9773 and 0.9481	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2620 / 0 / 299	
Goodness-of-fit on F^2	0.807	
Final R indices [I>2sigma(I)]	R1 = 0.0418, wR2 = 0.0939	
R indices (all data)	R1 = 0.0854, wR2 = 0.1034	
Absolute structure parameter	9(2)	
Extinction coefficient	0.0067(12)	
Largest diff. peak and hole	0.141 and -0.127 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **9g**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	-2866(4)	-4767(2)	-132(1)	46(1)
C(2)	-1996(5)	-4484(2)	401(2)	56(1)
C(3)	-2626(5)	-5165(2)	865(1)	53(1)
N(4)	-2850(4)	-6027(2)	523(1)	46(1)
C(5)	-4335(5)	-6597(2)	652(1)	51(1)
C(6)	-4696(5)	-7060(2)	64(1)	56(1)
C(7)	-4308(4)	-6306(2)	-399(1)	48(1)
C(7A)	-2824(4)	-5789(2)	-110(1)	47(1)
C(10)	-2068(5)	-4406(3)	-670(2)	61(1)
C(11)	-2156(5)	-3346(3)	-716(2)	55(1)
C(12)	-3438(5)	-2926(3)	-1008(2)	66(1)
C(13)	-3555(6)	-1959(3)	-1059(2)	77(1)
C(14)	-2355(7)	-1421(3)	-802(2)	83(2)
C(15)	-1074(7)	-1820(3)	-501(2)	83(1)
C(16)	-956(6)	-2779(3)	-467(2)	71(1)
C(31)	-1419(5)	-5254(3)	1377(2)	57(1)
C(32)	-1749(7)	-4821(3)	1906(2)	95(2)
C(33)	-534(9)	-4856(5)	2359(2)	115(2)
C(34)	916(9)	-5315(4)	2270(2)	114(2)
C(35)	1232(6)	-5745(4)	1755(2)	96(2)
C(36)	89(6)	-5724(3)	1309(2)	71(1)
C(51)	-3925(5)	-7308(3)	1136(2)	63(1)
O(51)	-3185(5)	-8023(2)	1058(1)	100(1)
O(52)	-4437(4)	-6998(2)	1654(1)	79(1)
C(52)	-4070(7)	-7515(4)	2213(2)	96(2)
C(53)	-2252(6)	-7609(4)	2297(2)	111(2)
C(54)	-4920(10)	-8460(5)	2179(3)	184(4)
C(55)	-4795(10)	-6876(6)	2668(2)	195(4)
C(71)	-3850(5)	-6750(3)	-997(2)	66(1)
O(71)	-6810(4)	-5536(2)	-67(1)	78(1)
O(72)	-5813(3)	-5186(2)	-958(1)	71(1)
C(72)	-5791(5)	-5645(3)	-436(2)	57(1)
C(73)	-7241(6)	-4550(3)	-1013(2)	107(2)

Table 3. Bond lengths [Å] and angles [°] for **9g**.

N(1)-C(2)	1.453(4)
N(1)-C(7A)	1.460(4)
N(1)-C(10)	1.470(4)
C(2)-C(3)	1.518(5)
C(3)-N(4)	1.465(4)
C(3)-C(31)	1.519(5)
N(4)-C(7A)	1.474(4)
N(4)-C(5)	1.475(4)
C(5)-C(6)	1.515(4)
C(5)-C(51)	1.530(5)
C(6)-C(7)	1.536(4)
C(7)-C(72)	1.524(5)
C(7)-C(71)	1.539(5)
C(7)-C(7A)	1.549(5)
C(10)-C(11)	1.519(5)
C(11)-C(12)	1.364(5)
C(11)-C(16)	1.381(5)
C(12)-C(13)	1.388(6)
C(13)-C(14)	1.364(6)
C(14)-C(15)	1.362(6)
C(15)-C(16)	1.375(6)
C(31)-C(32)	1.375(5)
C(31)-C(36)	1.394(5)
C(32)-C(33)	1.418(7)
C(33)-C(34)	1.353(7)
C(34)-C(35)	1.345(6)
C(35)-C(36)	1.366(5)
C(51)-O(51)	1.196(4)
C(51)-O(52)	1.319(4)
O(52)-C(52)	1.495(5)
C(52)-C(53)	1.481(7)
C(52)-C(55)	1.494(7)
C(52)-C(54)	1.515(8)
O(71)-C(72)	1.181(4)
O(72)-C(72)	1.350(4)
O(72)-C(73)	1.470(5)

C(2)-N(1)-C(7A)	103.8(3)
C(2)-N(1)-C(10)	112.4(3)
C(7A)-N(1)-C(10)	111.6(3)
N(1)-C(2)-C(3)	103.6(3)
N(4)-C(3)-C(31)	114.3(3)
N(4)-C(3)-C(2)	102.3(3)
C(31)-C(3)-C(2)	111.6(3)
C(3)-N(4)-C(7A)	108.5(2)
C(3)-N(4)-C(5)	117.3(3)
C(7A)-N(4)-C(5)	109.4(3)
N(4)-C(5)-C(6)	102.8(3)
N(4)-C(5)-C(51)	109.5(3)
C(6)-C(5)-C(51)	112.4(3)
C(5)-C(6)-C(7)	104.9(3)
C(72)-C(7)-C(6)	108.2(3)
C(72)-C(7)-C(71)	113.2(3)
C(6)-C(7)-C(71)	111.2(3)
C(72)-C(7)-C(7A)	109.4(3)
C(6)-C(7)-C(7A)	101.6(3)
C(71)-C(7)-C(7A)	112.6(3)
N(1)-C(7A)-N(4)	105.3(3)
N(1)-C(7A)-C(7)	116.3(3)
N(4)-C(7A)-C(7)	106.9(3)
N(1)-C(10)-C(11)	112.7(3)
C(12)-C(11)-C(16)	118.0(4)
C(12)-C(11)-C(10)	120.5(4)
C(16)-C(11)-C(10)	121.5(4)
C(11)-C(12)-C(13)	121.9(4)
C(14)-C(13)-C(12)	118.5(4)
C(13)-C(14)-C(15)	120.9(4)
C(14)-C(15)-C(16)	119.9(5)
C(15)-C(16)-C(11)	120.8(4)
C(32)-C(31)-C(36)	118.8(4)
C(32)-C(31)-C(3)	120.3(4)
C(36)-C(31)-C(3)	120.8(3)
C(31)-C(32)-C(33)	118.8(5)
C(34)-C(33)-C(32)	120.3(5)
C(35)-C(34)-C(33)	120.9(5)
C(34)-C(35)-C(36)	120.3(5)

C(35)-C(36)-C(31)	121.0(4)
O(51)-C(51)-O(52)	125.0(4)
O(51)-C(51)-C(5)	124.6(4)
O(52)-C(51)-C(5)	110.3(4)
C(51)-O(52)-C(52)	121.7(3)
C(53)-C(52)-O(52)	110.4(4)
C(53)-C(52)-C(55)	110.7(5)
O(52)-C(52)-C(55)	101.9(4)
C(53)-C(52)-C(54)	111.8(5)
O(52)-C(52)-C(54)	107.8(4)
C(55)-C(52)-C(54)	113.7(6)
C(72)-O(72)-C(73)	112.6(3)
O(71)-C(72)-O(72)	123.1(4)
O(71)-C(72)-C(7)	125.9(4)
O(72)-C(72)-C(7)	111.0(3)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **9g**. 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}
N(1)	53(2)	41(2)	42(2)	3(1)	-1(2)	-4(2)
C(2)	63(2)	49(2)	55(2)	3(2)	-4(2)	-1(2)
C(3)	62(3)	51(2)	47(2)	-7(2)	0(2)	1(2)
N(4)	51(2)	51(2)	35(2)	-1(1)	1(2)	-1(2)
C(5)	53(2)	50(2)	51(2)	7(2)	-2(2)	1(2)
C(6)	53(2)	56(2)	59(2)	1(2)	-4(2)	-11(2)
C(7)	47(2)	50(2)	46(2)	-2(2)	-7(2)	-3(2)
C(7A)	47(2)	56(2)	39(2)	4(2)	2(2)	1(2)
C(10)	64(3)	58(2)	61(2)	-2(2)	6(2)	-9(2)
C(11)	60(3)	55(2)	50(2)	11(2)	0(2)	-5(2)
C(12)	66(3)	74(3)	57(2)	2(2)	-1(2)	-2(2)
C(13)	83(4)	79(3)	70(3)	12(3)	2(3)	16(3)
C(14)	105(4)	63(3)	80(3)	13(3)	18(3)	10(3)
C(15)	96(4)	66(3)	87(3)	8(3)	0(3)	-19(3)
C(16)	67(3)	69(3)	76(3)	15(2)	-9(2)	-9(3)
C(31)	76(3)	53(2)	43(2)	-5(2)	0(2)	-13(2)
C(32)	121(4)	107(4)	56(2)	-29(3)	5(3)	-3(4)
C(33)	147(5)	143(5)	55(3)	-40(3)	-16(4)	-8(5)
C(34)	141(6)	120(5)	81(4)	-1(4)	-37(4)	-6(5)
C(35)	97(4)	110(4)	82(3)	1(3)	-24(3)	2(3)
C(36)	78(3)	74(3)	61(2)	-3(2)	-18(3)	1(3)
C(51)	62(3)	73(3)	54(3)	7(2)	8(2)	0(3)
O(51)	149(3)	80(2)	70(2)	12(2)	11(2)	33(2)
O(52)	81(2)	107(2)	50(2)	21(2)	12(2)	28(2)
C(52)	93(4)	142(5)	54(3)	32(3)	12(3)	29(4)
C(53)	109(4)	146(5)	78(3)	39(3)	-11(3)	25(4)
C(54)	169(6)	249(8)	135(5)	127(6)	-25(5)	-91(7)
C(55)	213(7)	318(10)	54(3)	24(5)	38(4)	144(8)
C(71)	75(3)	73(3)	51(2)	-8(2)	-7(2)	-10(2)
O(71)	67(2)	95(2)	71(2)	-4(2)	5(2)	12(2)
O(72)	63(2)	81(2)	70(2)	12(2)	-14(2)	7(2)
C(72)	56(3)	66(3)	48(2)	1(2)	-8(2)	-12(2)
C(73)	85(3)	115(4)	119(4)	17(3)	-27(3)	46(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **9g**.

	x	y	z	U(eq)
H(2A)	-2265	-3843	506	67
H(2B)	-802	-4539	351	67
H(3A)	-3706	-4951	1012	64
H(5A)	-5266	-6197	773	62
H(6A)	-5850	-7251	41	67
H(6B)	-3995	-7605	8	67
H(7AA)	-1783	-6013	-286	57
H(10A)	-2605	-4680	-1013	73
H(10B)	-912	-4598	-674	73
H(12A)	-4258	-3297	-1178	79
H(13A)	-4431	-1685	-1264	93
H(14A)	-2414	-772	-833	99
H(15A)	-281	-1445	-318	99
H(16A)	-56	-3049	-273	85
H(32A)	-2751	-4510	1966	114
H(33A)	-734	-4562	2719	138
H(34A)	1704	-5333	2571	137
H(35A)	2234	-6059	1701	115
H(36A)	319	-6026	954	85
H(53A)	-1756	-6999	2318	167
H(53B)	-1786	-7948	1970	167
H(53C)	-2035	-7943	2657	167
H(54A)	-4396	-8834	1880	277
H(54B)	-6072	-8374	2082	277
H(54C)	-4831	-8771	2553	277
H(55A)	-4203	-6293	2667	293
H(55B)	-4704	-7162	3051	293
H(55C)	-5945	-6764	2579	293
H(71A)	-4806	-7061	-1158	99
H(71B)	-2972	-7196	-941	99
H(71C)	-3487	-6270	-1264	99
H(73A)	-7202	-4241	-1389	160
H(73B)	-7201	-4091	-703	160
H(73C)	-8254	-4902	-982	160

Crystallographic data tables for compound **13a** (compound reference code OU2JSS)

Table 1. Crystal data and structure refinement for OU3ISS at 150.0(2) K.

Empirical formula	C 26 H 32 N 2 O 4
Formula weight	436.54
Crystal description	colourless plate
Crystal size	0.46 x 0.19 x 0.08 mm
Crystal system	Monoclinic
Space group	P2(1)
Unit cell dimensions	a = 10.276(2) A alpha = 90 deg. b = 5.799(3) A beta = 103.07(2) deg. c = 20.259(5) A gamma = 90 deg.
Volume	1176.0(7) A^3
Reflections for cell refinement	34
Range in theta	8.0 to 12.5 deg.
Z	2
Density (calculated)	1.233 Mg/m^3
Absorption coefficient	0.083 mm^-1
F(000)	468
Diffractometer type	Stoe Stadi-4 four-circle
Wavelength	0.71073 A
Scan type	omega-2theta
Reflections collected	2820
Theta range for data collection	2.55 to 25.05 deg.
Index ranges	-12<=h<=12, 0<=k<=6, -24<=l<=24
Independent reflections	2284 [R(int) = 0.072]
Observed reflections	1639 [I>2sigma(I)]
Decay correction	variation +/-6%
Structure solution by	direct methods
Hydrogen atom location	calculated
Hydrogen atom treatment	riding model
Data / restraints / parameters	2284/17/284 (least-squares on F^2)
Final R indices [I>2sigma(I)]	R1 = 0.0734, wR2 = 0.1170
Final R indices (all data)	R1 = 0.1226, wR2 = 0.1465
Goodness-of-fit on F^2	1.253

Absolute structure parameter	1(4)
Extinction coefficient	0.0054(12)
Final maximum delta/sigma	0.001

Weighting scheme
calc w=1/[\s^2^(Fo^2^)+2.20P] where P=(Fo^2^+2Fc^2^)/3

Largest diff. peak and hole	0.30 and -0.29 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for OU2JSS. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N1	1979(5)	3844(12)	3493(3)	23(1)
C2	3240(7)	2862(15)	3394(3)	26(2)
C3	2910(6)	2359(15)	2635(3)	24(2)
N4	2090(5)	4377(12)	2365(3)	22(2)
C5	1091(6)	3987(14)	1722(3)	21(2)
C6	-183(7)	5164(16)	1838(3)	28(2)
C7	-105(7)	4852(14)	2602(4)	25(2)
C7A	1412(6)	5216(14)	2887(3)	21(2)
C	2120(4)	5253(9)	4116(2)	32(2)
C11P	2502(4)	3638(9)	4738(2)	31(2)
C12P	3661(4)	4040(9)	5231(2)	34(2)
C13P	3966(7)	2622(12)	5806(3)	38(2)
C14P	3126(6)	832(14)	5883(4)	40(2)
C15P	1966(7)	446(15)	5395(3)	40(2)
C16P	1671(7)	1859(13)	4823(3)	37(2)
C31P	4108(6)	2091(10)	2320(3)	25(2)
C32P	4294(6)	73(14)	1991(3)	32(2)
C33P	5391(7)	-170(16)	1696(3)	42(2)
C34P	6294(7)	1619(12)	1736(3)	40(3)
C35P	6112(6)	3651(17)	2064(3)	36(2)
C36P	5010(6)	3877(15)	2355(3)	31(2)
O51	1647(5)	7180(10)	1065(2)	30(1)
C51	1566(7)	5129(16)	1134(3)	22(2)
O52	1869(5)	3494(10)	727(2)	29(1)
C52	2346(7)	4146(15)	104(3)	27(2)
C53	2569(9)	1778(17)	-172(4)	44(2)
C54	3648(6)	5426(16)	310(4)	33(2)
C55	1249(7)	5464(17)	-369(3)	35(2)
O71	-349(5)	723(10)	2489(2)	30(1)
C71	-514(7)	2485(15)	2769(3)	24(2)
O72	-1115(5)	2550(10)	3300(2)	30(1)
C72	-1583(8)	340(17)	3483(4)	40(2)

Table 3. Selected bond lengths [A], angles and torsions [deg] for OU2JSS.

N1-C2	1.470(8)
N1-C	1.483(7)
N1-C7A	1.469(8)
C2-C3	1.526(9)
C3-N4	1.473(9)
C3-C31P	1.517(9)
N4-C7A	1.475(8)
N4-C5	1.482(8)
C5-C51	1.534(9)
C5-C6	1.541(9)
C6-C7	1.543(9)
C7-C71	1.496(11)
C7-C7A	1.550(9)
C-C11P	1.547(9)
O51-C51	1.202(10)
C51-O52	1.339(9)
O52-C52	1.503(8)
C52-C54	1.504(10)
C52-C55	1.511(10)
C52-C53	1.519(12)
O71-C71	1.199(9)
C71-O72	1.357(8)
O72-C72	1.447(10)
C7A-N1-C2	106.9(5)
C7A-N1-C	110.9(5)
C2-N1-C	114.2(5)
N1-C2-C3	102.1(5)
N4-C3-C31P	112.0(6)
N4-C3-C2	101.6(6)
C31P-C3-C2	115.2(5)
C3-N4-C7A	108.5(5)
C3-N4-C5	115.5(6)
C7A-N4-C5	109.6(5)
N4-C5-C51	109.7(5)
N4-C5-C6	104.0(5)
C51-C5-C6	110.9(6)
C5-C6-C7	104.4(5)
C71-C7-C6	112.3(7)
C71-C7-C7A	110.6(6)
C6-C7-C7A	100.2(5)
N1-C7A-N4	105.0(6)
N1-C7A-C7	114.4(5)
N4-C7A-C7	106.7(5)
N1-C-C11P	108.5(3)
C16P-C11P-C	120.4(3)
C12P-C11P-C	120.1(3)
C32P-C31P-C3	120.3(6)
C36P-C31P-C3	120.1(6)
O51-C51-O52	126.6(7)
O51-C51-C5	124.1(7)
O52-C51-C5	109.3(7)
C51-O52-C52	120.3(6)
O52-C52-C54	109.3(5)
O52-C52-C55	108.7(5)
C54-C52-C55	114.5(7)
O52-C52-C53	100.8(6)
C54-C52-C53	110.5(6)
C55-C52-C53	112.1(7)

O71-C71-O72	122.5(7)
O71-C71-C7	126.8(6)
O72-C71-C7	110.7(7)
C71-O72-C72	114.6(6)

Table 4. Bond lengths [A], angles and torsions [deg] for OU2JSS.

N1-C7A	1.469(8)
N1-C2	1.470(8)
N1-C	1.483(7)
C2-C3	1.526(9)
C3-N4	1.473(9)
C3-C31P	1.517(9)
N4-C7A	1.475(8)
N4-C5	1.482(8)
C5-C51	1.534(9)
C5-C6	1.541(9)
C6-C7	1.543(9)
C7-C71	1.496(11)
C7-C7A	1.550(9)
C-C11P	1.547(9)
C11P-C16P	1.375(7)
C11P-C12P	1.390(7)
C12P-C13P	1.403(8)
C13P-C14P	1.381(9)
C14P-C15P	1.384(8)
C15P-C16P	1.396(8)
C31P-C32P	1.381(8)
C31P-C36P	1.382(8)
C32P-C33P	1.397(8)
C33P-C34P	1.382(9)
C34P-C35P	1.386(9)
C35P-C36P	1.395(8)
O51-C51	1.202(10)
C51-O52	1.339(9)
O52-C52	1.503(8)
C52-C54	1.504(10)
C52-C55	1.511(10)
C52-C53	1.519(12)
O71-C71	1.199(9)
C71-O72	1.357(8)
O72-C72	1.447(10)

C7A-N1-C2	106.9(5)
C7A-N1-C	110.9(5)
C2-N1-C	114.2(5)
N1-C2-C3	102.1(5)
N4-C3-C31P	112.0(6)
N4-C3-C2	101.6(6)
C31P-C3-C2	115.2(5)
C3-N4-C7A	108.5(5)
C3-N4-C5	115.5(6)
C7A-N4-C5	109.6(5)
N4-C5-C51	109.7(5)
N4-C5-C6	104.0(5)
C51-C5-C6	110.9(6)
C5-C6-C7	104.4(5)
C71-C7-C6	112.3(7)
C71-C7-C7A	110.6(6)
C6-C7-C7A	100.2(5)
N1-C7A-N4	105.0(6)
N1-C7A-C7	114.4(5)
N4-C7A-C7	106.7(5)
N1-C-C11P	108.5(3)
C16P-C11P-C12P	119.4(3)
C16P-C11P-C	120.4(3)

C12P-C11P-C	120.1(5)
C11P-C12P-C13P	119.6(4)
C14P-C13P-C12P	120.4(6)
C13P-C14P-C15P	120.0(8)
C14P-C15P-C16P	119.2(7)
C11P-C16P-C15P	121.4(6)
C32P-C31P-C36P	119.7(7)
C32P-C31P-C3	120.3(6)
C36P-C31P-C3	120.1(6)
C31P-C32P-C33P	120.4(7)
C34P-C33P-C32P	119.7(8)
C33P-C34P-C35P	120.3(7)
C34P-C35P-C36P	119.5(7)
C31P-C36P-C35P	120.5(7)
O51-C51-O52	126.6(7)
O51-C51-C5	124.1(7)
O52-C51-C5	109.3(7)
C51-O52-C52	120.3(6)
O52-C52-C54	109.3(5)
O52-C52-C55	108.7(5)
C54-C52-C55	114.5(7)
O52-C52-C53	100.8(6)
C54-C52-C53	110.5(6)
C55-C52-C53	112.1(7)
O71-C71-O72	122.5(7)
O71-C71-C7	126.8(6)
O72-C71-C7	110.7(7)
C71-O72-C72	114.6(6)
C7A-N1-C2-C3	-36.1(8)
C-N1-C2-C3	-159.2(6)
N1-C2-C3-N4	38.8(7)
N1-C2-C3-C31P	160.1(7)
C31P-C3-N4-C7A	-152.0(6)
C2-C3-N4-C7A	-28.5(7)
C31P-C3-N4-C5	84.5(7)
C2-C3-N4-C5	-151.9(5)
C3-N4-C5-C51	-105.8(7)
C7A-N4-C5-C51	131.3(6)
C3-N4-C5-C6	135.5(6)
C7A-N4-C5-C6	12.6(8)
N4-C5-C6-C7	-32.5(8)
C51-C5-C6-C7	-150.4(6)
C5-C6-C7-C71	-78.7(7)
C5-C6-C7-C7A	38.6(7)
C2-N1-C7A-N4	18.8(7)
C-N1-C7A-N4	143.9(5)
C2-N1-C7A-C7	135.4(7)
C-N1-C7A-C7	-99.5(7)
C3-N4-C7A-N1	6.9(7)
C5-N4-C7A-N1	133.8(6)
C3-N4-C7A-C7	-114.8(6)
C5-N4-C7A-C7	12.1(8)
C71-C7-C7A-N1	-28.2(9)
C6-C7-C7A-N1	-146.8(6)
C71-C7-C7A-N4	87.5(7)
C6-C7-C7A-N4	-31.2(8)
C7A-N1-C-C11P	171.0(4)
C2-N1-C-C11P	-68.1(6)
N1-C-C11P-C16P	-59.8(5)
N1-C-C11P-C12P	123.0(3)
C16P-C11P-C12P-C13P	0.1(4)
C-C11P-C12P-C13P	177.3(2)
C11P-C12P-C13P-C14P	0.3(4)

C12P-C13P-C14P-C15P	-0.9(8)
C13P-C14P-C15P-C16P	1.1(10)
C12P-C11P-C16P-C15P	0.1(8)
C-C11P-C16P-C15P	-177.1(5)
C14P-C15P-C16P-C11P	-0.7(10)
N4-C3-C31P-C32P	-122.9(6)
C2-C3-C31P-C32P	121.6(6)
N4-C3-C31P-C36P	56.4(7)
C2-C3-C31P-C36P	-59.1(9)
C36P-C31P-C32P-C33P	0.2(4)
C3-C31P-C32P-C33P	179.5(5)
C31P-C32P-C33P-C34P	0.2(4)
C32P-C33P-C34P-C35P	-0.3(8)
C33P-C34P-C35P-C36P	0.0(10)
C32P-C31P-C36P-C35P	-0.5(8)
C3-C31P-C36P-C35P	-179.7(6)
C34P-C35P-C36P-C31P	0.4(9)
N4-C5-C51-O51	-68.2(9)
C6-C5-C51-O51	46.1(9)
N4-C5-C51-O52	111.6(6)
C6-C5-C51-O52	-134.1(6)
O51-C51-O52-C52	-1.0(10)
C5-C51-O52-C52	179.2(5)
C51-O52-C52-C54	62.9(8)
C51-O52-C52-C55	-62.7(8)
C51-O52-C52-C53	179.2(6)
C6-C7-C71-O71	33.0(10)
C7A-C7-C71-O71	-78.0(9)
C6-C7-C71-O72	-147.3(6)
C7A-C7-C71-O72	101.7(6)
O71-C71-O72-C72	-2.2(10)
C7-C71-O72-C72	178.1(6)

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for OU2JSS. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N1	26(3)	24(4)	18(3)	3(3)	5(2)	-1(3)
C2	25(4)	31(5)	21(4)	1(4)	2(3)	5(4)
C3	19(3)	29(5)	23(4)	0(4)	3(3)	0(4)
N4	20(3)	30(4)	17(3)	-3(3)	6(2)	4(3)
C5	24(3)	19(4)	18(3)	-5(3)	2(3)	-6(4)
C6	28(4)	32(5)	24(4)	7(4)	4(3)	-1(4)
C7	22(4)	22(5)	33(4)	5(4)	9(3)	1(4)
C7A	24(4)	20(4)	19(3)	5(3)	5(3)	-5(4)
C	34(4)	33(5)	28(4)	3(4)	8(3)	3(4)
C11P	33(4)	39(5)	22(4)	-1(4)	9(3)	-9(4)
C12P	27(4)	44(6)	31(4)	-10(5)	10(3)	-5(4)
C13P	29(4)	56(6)	25(4)	6(5)	-2(3)	3(5)
C14P	37(5)	48(6)	32(4)	4(5)	0(4)	12(5)
C15P	44(5)	42(6)	34(4)	9(5)	8(4)	-5(5)
C16P	39(5)	45(6)	22(4)	4(4)	-5(3)	-14(5)
C31P	19(4)	35(5)	19(4)	1(4)	-1(3)	0(4)
C32P	26(4)	34(5)	33(4)	-8(4)	0(3)	-4(4)
C33P	31(4)	57(7)	38(5)	-13(5)	8(4)	5(5)
C34P	19(4)	74(8)	31(4)	-8(5)	10(3)	9(5)
C35P	21(4)	56(6)	30(4)	2(5)	5(3)	-1(5)
C36P	24(4)	46(5)	22(4)	-1(4)	6(3)	-4(4)
O51	37(3)	22(4)	31(3)	2(3)	10(2)	-6(3)
C51	19(4)	32(5)	14(3)	-4(4)	2(3)	-5(4)
O52	30(3)	37(4)	19(2)	1(3)	7(2)	-2(3)
C52	31(4)	32(5)	23(4)	2(4)	15(3)	-6(4)
C53	54(5)	47(6)	37(5)	-8(5)	21(4)	-1(5)
C54	26(4)	42(5)	31(4)	9(4)	8(3)	-1(4)
C55	33(4)	52(6)	20(4)	1(4)	7(3)	-6(5)
O71	38(3)	24(4)	32(3)	-6(3)	17(2)	-4(3)
C71	23(4)	25(5)	22(4)	-5(4)	3(3)	-2(4)
O72	33(3)	34(3)	25(3)	1(3)	15(2)	-4(3)
C72	49(5)	39(6)	39(5)	-2(5)	23(4)	-14(5)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for OU2JSS.

	x	y	z	U(eq)
H2A	3477	1434	3662	31
H2B	3983	3981	3518	31
H3A	2347	937	2545	28
H5A	937	2300	1636	25
H6A	-993	4415	1564	34
H6B	-196	6819	1717	34
H7A	-639	6060	2775	30
H7AA	1609	6889	2979	25
H0A	1267	6047	4117	38
H0B	2821	6436	4133	38
H12A	4243	5266	5178	40
H13A	4755	2895	6145	46
H14A	3345	-136	6271	48
H15A	1377	-767	5449	49
H16A	880	1585	4485	45
H32A	3674	-1156	1966	38
H33A	5515	-1558	1469	50
H34A	7043	1456	1538	49
H35A	6733	4881	2092	43
H36A	4880	5270	2578	37
H53A	3280	979	151	66
H53B	2829	1949	-606	66
H53C	1742	880	-239	66
H54A	4304	4456	613	49
H54B	3510	6850	545	49
H54C	3978	5805	-95	49
H55A	440	4514	-480	52
H55B	1536	5844	-785	52
H55C	1060	6889	-148	52
H72A	-1999	536	3870	60
H72B	-827	-725	3607	60
H72C	-2241	-287	3098	60

Crystallographic data tables for compound **19** (compound reference code JSPHNO)

Table 1. Crystal data and structure refinement for [redacted].

Identification code	JSPHNO
Empirical formula	C25 H28 N2 O4
Formula weight	420.49
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system	Monoclinic
Space group	P2(1)
Unit cell dimensions	a = 11.351(2) A alpha = 90 deg. b = 9.7612(10) A beta = 91.07(2) deg. c = 19.942(3) A gamma = 90 deg.
Volume	2209.1(5) A^3
Z	4
Density (calculated)	1.264 Mg/m^3
Absorption coefficient	0.086 mm^-1
F(000)	896
Crystal size	0.39 x 0.39 x 0.10 mm
Theta range for data collection	1.79 to 22.49 deg.
Index ranges	-12<=h<=12, 0<=k<=10, 0<=l<=21
Reflections collected	3081
Independent reflections	3081
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3072 / 33 / 548
Goodness-of-fit on F^2	1.006

Final R indices [I>2sigma(I)]	R1 = 0.0494, wR2 = 0.100
R indices (all data)	R1 = 0.0936, wR2 = 0.141
Absolute structure parameter	not reliably determined
Extinction coefficient	0.0071(12)
Largest diff. peak and hole	0.16 and -0.14 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for JSPHNO. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	-803(4)	-4772(5)	1411(2)	47(1)
C(2)	264(5)	-5582(7)	1471(4)	58(2)
C(3)	1230(5)	-4643(7)	1208(3)	46(2)
N(4)	819(4)	-3279(5)	1409(2)	42(1)
C(5)	944(5)	-2132(7)	928(3)	52(2)
C(6)	-104(5)	-1211(7)	1055(3)	58(2)
C(7)	-1091(6)	-2225(7)	1224(3)	57(2)
C(7A)	-431(5)	-3375(7)	1599(3)	47(2)
C(8)	2171(7)	-1517(8)	1037(4)	58(2)
O(8)	3040(4)	-2042(6)	817(3)	83(2)
O(9)	2275(4)	-393(6)	1415(3)	81(2)
C(10)	1281(7)	484(9)	1524(4)	86(3)
C(11)	178(6)	-245(8)	1641(4)	75(2)
C	-1735(3)	-5282(5)	1846(2)	58(2)
C(11P)	-2146(3)	-6690(5)	1636(2)	51(2)
C(12P)	-2457(3)	-7654(5)	2115(2)	59(2)
C(13P)	-2918(6)	-8906(8)	1934(4)	74(2)
C(14P)	-3088(6)	-9232(9)	1271(4)	74(2)
C(15P)	-2756(7)	-8299(9)	794(4)	75(2)
C(16P)	-2299(6)	-7052(8)	978(4)	67(2)
C(31P)	2414(5)	-5097(7)	1484(3)	49(2)
C(32P)	2940(5)	-4514(8)	2034(3)	66(2)
C(33P)	3944(6)	-5077(8)	2332(4)	69(2)
C(34P)	4426(6)	-6243(9)	2079(4)	80(3)
C(35P)	3910(7)	-6837(10)	1534(5)	98(3)
C(36P)	2912(6)	-6271(9)	1248(4)	77(2)
C(71)	-1722(6)	-2775(8)	609(4)	59(2)
O(71)	-1282(4)	-2882(7)	68(3)	87(2)
O(72)	-2822(4)	-3105(5)	744(2)	67(1)
C(72)	-3536(7)	-3714(11)	200(4)	92(3)
C(73)	-4615(7)	-4258(15)	456(5)	142(5)
N(1')	-2463(4)	-166(5)	4315(2)	49(1)

C(2')	-1489(5)	178(7)	3871(3)	58(2)
C(3')	-814(5)	1246(7)	4278(3)	46(2)
N(4')	-866(4)	687(6)	4959(3)	51(1)
C(5')	-907(5)	1679(8)	5494(3)	59(2)
C(6')	-2213(5)	1908(8)	5639(3)	56(2)
C(7')	-2699(5)	438(7)	5552(3)	53(2)
C(7A')	-1934(5)	-202(7)	4998(3)	51(2)
C(8')	-199(8)	1263(11)	6118(5)	82(3)
O(8')	548(6)	396(8)	6126(3)	113(2)
O(9')	-466(7)	1936(9)	6687(3)	112(2)
C(10')	-1370(10)	3001(13)	6659(5)	116(4)
C(11')	-2458(8)	2525(10)	6323(4)	90(3)
C'	-3039(3)	-1469(5)	4144(2)	64(2)
C(1B')	-3709(3)	-1416(5)	3491(2)	56(2)
C(12')	-4646(3)	-517(5)	3393(2)	66(2)
C(13')	-5290(6)	-540(9)	2796(4)	75(2)
C(14')	-5020(7)	-1421(9)	2293(4)	70(2)
C(15')	-4090(7)	-2287(9)	2378(4)	79(2)
C(16')	-3443(6)	-2276(8)	2971(4)	75(2)
C(31')	413(5)	1519(7)	4044(3)	48(2)
C(32')	591(6)	2261(8)	3468(4)	63(2)
C(33')	1702(6)	2531(8)	3229(4)	68(2)
C(34')	2669(6)	2063(8)	3584(4)	66(2)
C(35')	2533(6)	1339(8)	4171(4)	65(2)
C(36')	1407(5)	1066(7)	4397(3)	60(2)
C(71')	-4007(6)	466(9)	5416(3)	57(2)
O(71')	-4520(4)	1278(7)	5083(3)	93(2)
O(72')	-4546(4)	-547(6)	5724(2)	74(2)
C(72')	-5836(6)	-591(11)	5661(4)	94(3)
C(73')	-6333(7)	-1258(14)	6201(5)	128(4)

Table 3. Selected bond lengths [A] and angles [deg] for JSPHNO

N(1)-C(2)	1.450(8)
N(1)-C	1.467(6)
N(1)-C(7A)	1.473(8)
C(2)-C(3)	1.529(9)
C(3)-N(4)	1.469(8)
C(3)-C(31P)	1.508(8)
N(4)-C(7A)	1.477(7)
N(4)-C(5)	1.484(8)
C(5)-C(6)	1.516(9)
C(5)-C(8)	1.529(9)
C(6)-C(11)	1.532(9)
C(6)-C(7)	1.537(9)
C(7)-C(71)	1.506(9)
C(7)-C(7A)	1.536(9)
C(8)-O(8)	1.202(8)
C(8)-O(9)	1.335(9)

O(9)-C(10)	1.436(8)
C(10)-C(11)	1.463(10)
C-C(11P)	1.508(11)
C(71)-O(71)	1.203(7)
C(71)-O(72)	1.322(8)
O(72)-C(72)	1.468(8)
C(72)-C(73)	1.438(10)
N(1')-C'	1.468(6)
N(1')-C(2')	1.468(7)
N(1')-C(7A')	1.478(7)
C(2')-C(3')	1.519(8)
C(3')-N(4')	1.466(7)
C(3')-C(31')	1.501(8)
N(4')-C(5')	1.444(8)
N(4')-C(7A')	1.494(7)
C(5')-C(8')	1.523(10)
C(5')-C(6')	1.532(9)
C(6')-C(11')	1.521(10)
C(6')-C(7')	1.545(9)
C(7')-C(71')	1.505(8)
C(7')-C(7A')	1.550(9)
C(8')-O(8')	1.198(11)
C(8')-O(9')	1.352(11)
O(9')-C(10')	1.461(12)
C(10')-C(11')	1.470(11)
C'-C(1B')	1.50(2)

C(2)-N(1)-C	112.1(5)
C(2)-N(1)-C(7A)	104.4(5)
C-N(1)-C(7A)	111.8(5)
N(1)-C(2)-C(3)	104.4(5)
N(4)-C(3)-C(31P)	116.9(5)
N(4)-C(3)-C(2)	102.5(5)
C(31P)-C(3)-C(2)	109.8(5)
C(3)-N(4)-C(7A)	108.9(5)
C(3)-N(4)-C(5)	118.2(5)
C(7A)-N(4)-C(5)	108.5(5)
N(4)-C(5)-C(6)	104.7(5)
N(4)-C(5)-C(8)	107.6(5)
C(6)-C(5)-C(8)	117.3(6)
C(5)-C(6)-C(11)	109.8(5)
C(5)-C(6)-C(7)	103.4(5)
C(11)-C(6)-C(7)	111.8(6)
C(71)-C(7)-C(7A)	110.8(6)
C(71)-C(7)-C(6)	112.9(6)
C(7A)-C(7)-C(6)	103.1(5)
N(1)-C(7A)-N(4)	105.4(5)
N(1)-C(7A)-C(7)	114.7(5)
N(4)-C(7A)-C(7)	106.9(5)
O(8)-C(8)-O(9)	119.5(7)
O(8)-C(8)-C(5)	122.2(7)
O(9)-C(8)-C(5)	118.3(7)

C(8)-O(9)-C(10)	121.0(6)
O(9)-C(10)-C(11)	114.3(7)
C(10)-C(11)-C(6)	110.1(6)
N(1)-C-C(11P)	111.6(3)
C(32P)-C(31P)-C(3)	122.9(6)
C(36P)-C(31P)-C(3)	119.6(6)
O(71)-C(71)-O(72)	124.7(6)
O(71)-C(71)-C(7)	124.3(7)
O(72)-C(71)-C(7)	111.0(6)
C(71)-O(72)-C(72)	117.3(6)
C(73)-C(72)-O(72)	110.4(6)
C'-N(1')-C(2')	113.3(4)
C'-N(1')-C(7A')	111.5(4)
C(2')-N(1')-C(7A')	105.3(4)
N(1')-C(2')-C(3')	102.3(5)
N(4')-C(3')-C(31')	114.0(5)
N(4')-C(3')-C(2')	102.1(5)
C(31')-C(3')-C(2')	114.7(5)
C(5')-N(4')-C(3')	116.0(5)
C(5')-N(4')-C(7A')	108.3(5)
C(3')-N(4')-C(7A')	108.1(4)
N(4')-C(5')-C(8')	113.6(7)
N(4')-C(5')-C(6')	106.4(5)
C(8')-C(5')-C(6')	112.5(6)
C(11')-C(6')-C(5')	114.9(6)
C(11')-C(6')-C(7')	113.5(6)
C(5')-C(6')-C(7')	100.8(6)
C(71')-C(7')-C(6')	110.6(6)
C(71')-C(7')-C(7A')	116.3(5)
C(6')-C(7')-C(7A')	104.6(5)
N(1')-C(7A')-N(4')	104.7(5)
N(1')-C(7A')-C(7')	115.1(5)
N(4')-C(7A')-C(7')	105.6(5)
O(8')-C(8')-O(9')	120.1(9)
O(8')-C(8')-C(5')	124.2(10)
O(9')-C(8')-C(5')	115.7(9)
C(8')-O(9')-C(10')	118.8(7)
O(9')-C(10')-C(11')	112.1(9)
C(10')-C(11')-C(6')	111.6(7)
N(1')-C'-C(1B')	112.9(2)
C(16')-C(1B')-C(12')	117.3(4)
C(16')-C(1B')-C'	121.4(4)
C(12')-C(1B')-C'	121.2(4)
C(32')-C(31')-C(3')	120.3(5)
C(36')-C(31')-C(3')	122.3(6)
O(71')-C(71')-C(7')	126.0(7)
O(72')-C(71')-C(7')	111.5(6)
C(71')-O(72')-C(72')	116.8(6)
C(73')-C(72')-O(72')	111.4(7)

Table 4. Bond lengths [A] and angles [deg] for JSPHNO

N(1)-C(2)	1.450(8)
N(1)-C	1.467(6)
N(1)-C(7A)	1.473(8)
C(2)-C(3)	1.529(9)
C(3)-N(4)	1.469(8)
C(3)-C(31P)	1.508(8)
N(4)-C(7A)	1.477(7)
N(4)-C(5)	1.484(8)
C(5)-C(6)	1.516(9)
C(5)-C(8)	1.529(9)
C(6)-C(11)	1.532(9)
C(6)-C(7)	1.537(9)
C(7)-C(71)	1.506(9)
C(7)-C(7A)	1.536(9)
C(8)-O(8)	1.202(8)
C(8)-O(9)	1.335(9)
O(9)-C(10)	1.436(8)
C(10)-C(11)	1.463(10)
C-C(11P)	1.508(11)
C(11P)-C(16P)	1.368(8)
C(11P)-C(12P)	1.390(11)
C(12P)-C(13P)	1.375(9)
C(13P)-C(14P)	1.371(9)
C(14P)-C(15P)	1.374(10)
C(15P)-C(16P)	1.370(9)
C(31P)-C(32P)	1.364(8)
C(31P)-C(36P)	1.365(9)
C(32P)-C(33P)	1.389(8)
C(33P)-C(34P)	1.364(9)
C(34P)-C(35P)	1.356(10)
C(35P)-C(36P)	1.375(9)
C(71)-O(71)	1.203(7)
C(71)-O(72)	1.322(8)
O(72)-C(72)	1.468(8)
C(72)-C(73)	1.438(10)
N(1')-C'	1.468(6)
N(1')-C(2')	1.468(7)
N(1')-C(7A')	1.478(7)
C(2')-C(3')	1.519(8)
C(3')-N(4')	1.466(7)
C(3')-C(31')	1.501(8)
N(4')-C(5')	1.444(8)
N(4')-C(7A')	1.494(7)
C(5')-C(8')	1.523(10)
C(5')-C(6')	1.532(9)
C(6')-C(11')	1.521(10)
C(6')-C(7')	1.545(9)
C(7')-C(71')	1.505(8)
C(7')-C(7A')	1.550(9)
C(8')-O(8')	1.198(11)

C(8')-O(9')	1.352(11)
O(9')-C(10')	1.461(12)
C(10')-C(11')	1.470(11)
C'-C(1B')	1.50(2)
C(1B')-C(16')	1.371(8)
C(1B')-C(12')	1.39(2)
C(12')-C(13')	1.385(7)
C(13')-C(14')	1.361(9)
C(14')-C(15')	1.360(9)
C(15')-C(16')	1.381(9)
C(31')-C(32')	1.376(8)
C(31')-C(36')	1.391(8)
C(32')-C(33')	1.381(8)
C(33')-C(34')	1.373(9)
C(34')-C(35')	1.380(9)
C(35')-C(36')	1.388(8)
C(71')-O(71')	1.180(8)
C(71')-O(72')	1.321(8)
O(72')-C(72')	1.468(7)
C(72')-C(73')	1.389(11)

C(2)-N(1)-C	112.1(5)
C(2)-N(1)-C(7A)	104.4(5)
C-N(1)-C(7A)	111.8(5)
N(1)-C(2)-C(3)	104.4(5)
N(4)-C(3)-C(31P)	116.9(5)
N(4)-C(3)-C(2)	102.5(5)
C(31P)-C(3)-C(2)	109.8(5)
C(3)-N(4)-C(7A)	108.9(5)
C(3)-N(4)-C(5)	118.2(5)
C(7A)-N(4)-C(5)	108.5(5)
N(4)-C(5)-C(6)	104.7(5)
N(4)-C(5)-C(8)	107.6(5)
C(6)-C(5)-C(8)	117.3(6)
C(5)-C(6)-C(11)	109.8(5)
C(5)-C(6)-C(7)	103.4(5)
C(11)-C(6)-C(7)	111.8(6)
C(71)-C(7)-C(7A)	110.8(6)
C(71)-C(7)-C(6)	112.9(6)
C(7A)-C(7)-C(6)	103.1(5)
N(1)-C(7A)-N(4)	105.4(5)
N(1)-C(7A)-C(7)	114.7(5)
N(4)-C(7A)-C(7)	106.9(5)
O(8)-C(8)-O(9)	119.5(7)
O(8)-C(8)-C(5)	122.2(7)
O(9)-C(8)-C(5)	118.3(7)
C(8)-O(9)-C(10)	121.0(6)
O(9)-C(10)-C(11)	114.3(7)
C(10)-C(11)-C(6)	110.1(6)
N(1)-C-C(11P)	111.6(3)
C(16P)-C(11P)-C(12P)	117.0(4)
C(16P)-C(11P)-C	122.3(4)

C(12P)-C(11P)-C	120.5(4)
C(13P)-C(12P)-C(11P)	121.5(4)
C(14P)-C(13P)-C(12P)	120.3(7)
C(13P)-C(14P)-C(15P)	118.6(8)
C(16P)-C(15P)-C(14P)	120.7(7)
C(11P)-C(16P)-C(15P)	121.8(7)
C(32P)-C(31P)-C(36P)	116.7(6)
C(32P)-C(31P)-C(3)	122.9(6)
C(36P)-C(31P)-C(3)	119.6(6)
C(31P)-C(32P)-C(33P)	121.5(7)
C(34P)-C(33P)-C(32P)	120.3(7)
C(35P)-C(34P)-C(33P)	118.9(7)
C(34P)-C(35P)-C(36P)	120.0(8)
C(31P)-C(36P)-C(35P)	122.6(7)
O(71)-C(71)-O(72)	124.7(6)
O(71)-C(71)-C(7)	124.3(7)
O(72)-C(71)-C(7)	111.0(6)
C(71)-O(72)-C(72)	117.3(6)
C(73)-C(72)-O(72)	110.4(6)
C'-N(1')-C(2')	113.3(4)
C'-N(1')-C(7A')	111.5(4)
C(2')-N(1')-C(7A')	105.3(4)
N(1')-C(2')-C(3')	102.3(5)
N(4')-C(3')-C(31')	114.0(5)
N(4')-C(3')-C(2')	102.1(5)
C(31')-C(3')-C(2')	114.7(5)
C(5')-N(4')-C(3')	116.0(5)
C(5')-N(4')-C(7A')	108.3(5)
C(3')-N(4')-C(7A')	108.1(4)
N(4')-C(5')-C(8')	113.6(7)
N(4')-C(5')-C(6')	106.4(5)
C(8')-C(5')-C(6')	112.5(6)
C(11')-C(6')-C(5')	114.9(6)
C(11')-C(6')-C(7')	113.5(6)
C(5')-C(6')-C(7')	100.8(6)
C(71')-C(7')-C(6')	110.6(6)
C(71')-C(7')-C(7A')	116.3(5)
C(6')-C(7')-C(7A')	104.6(5)
N(1')-C(7A')-N(4')	104.7(5)
N(1')-C(7A')-C(7')	115.1(5)
N(4')-C(7A')-C(7')	105.6(5)
O(8')-C(8')-O(9')	120.1(9)
O(8')-C(8')-C(5')	124.2(10)
O(9')-C(8')-C(5')	115.7(9)
C(8')-O(9')-C(10')	118.8(7)
O(9')-C(10')-C(11')	112.1(9)
C(10')-C(11')-C(6')	111.6(7)
N(1')-C'-C(1B')	112.9(2)
C(16')-C(1B')-C(12')	117.3(4)
C(16')-C(1B')-C'	121.4(4)
C(12')-C(1B')-C'	121.2(4)
C(13')-C(12')-C(1B')	120.0(4)

C(14')-C(13')-C(12')	121.5(7)
C(15')-C(14')-C(13')	119.0(7)
C(14')-C(15')-C(16')	120.1(8)
C(1B')-C(16')-C(15')	122.1(7)
C(32')-C(31')-C(36')	117.3(6)
C(32')-C(31')-C(3')	120.3(5)
C(36')-C(31')-C(3')	122.3(6)
C(31')-C(32')-C(33')	122.5(6)
C(34')-C(33')-C(32')	119.0(7)
C(33')-C(34')-C(35')	120.4(7)
C(34')-C(35')-C(36')	119.5(6)
O(71')-C(71')-C(7')	126.0(7)
O(72')-C(71')-C(7')	111.5(6)
C(71')-O(72')-C(72')	116.8(6)
C(73')-C(72')-O(72')	111.4(7)

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for JSPHNO. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(1)	40(3)	50(4)	52(3)	0(3)	5(2)	-2(3)
C(2)	51(4)	45(4)	79(5)	3(4)	-1(4)	3(4)
C(3)	42(4)	46(4)	51(4)	0(4)	-2(3)	7(3)
N(4)	43(3)	37(3)	47(3)	3(3)	2(2)	1(3)
C(5)	59(4)	52(5)	45(4)	-2(4)	-9(3)	-10(4)
C(6)	56(4)	53(5)	63(4)	3(4)	-16(3)	15(4)
C(7)	53(4)	60(5)	58(4)	-10(4)	-16(3)	10(4)
C(7A)	50(4)	39(4)	50(4)	-3(4)	0(3)	4(3)
C(8)	61(5)	58(5)	55(5)	10(4)	-8(4)	-12(4)
O(8)	54(3)	95(5)	99(4)	-13(4)	10(3)	1(3)
O(9)	65(3)	61(4)	116(4)	-26(4)	-13(3)	-7(3)
C(10)	82(6)	58(5)	119(7)	-29(5)	0(5)	4(5)
C(11)	73(5)	54(5)	99(6)	-18(5)	2(4)	-9(5)
C	61(4)	53(5)	60(4)	-2(4)	6(3)	3(4)
C(11P)	41(4)	51(5)	60(5)	3(4)	3(3)	1(3)
C(12P)	51(4)	66(6)	61(4)	9(5)	2(3)	-1(4)
C(13P)	58(5)	69(6)	95(6)	21(5)	9(4)	-10(5)
C(14P)	61(5)	56(6)	106(7)	11(6)	-2(5)	-9(4)
C(15P)	78(5)	72(6)	74(6)	-11(5)	-7(4)	-11(5)
C(16P)	73(5)	58(5)	69(6)	15(5)	5(4)	-6(4)
C(31P)	38(4)	42(4)	67(4)	-9(4)	2(3)	-2(3)
C(32P)	59(4)	61(5)	78(5)	-14(5)	-13(4)	15(4)
C(33P)	59(5)	78(6)	69(5)	0(5)	-21(4)	7(4)
C(34P)	46(4)	84(7)	110(7)	-11(6)	-12(4)	24(5)
C(35P)	69(5)	88(7)	137(8)	-44(7)	-23(5)	27(5)
C(36P)	63(5)	82(6)	86(6)	-39(5)	-24(4)	15(5)

C(71)	50(4)	62(5)	63(5)	10(5)	-9(4)	2(4)
O(71)	67(3)	136(6)	56(3)	12(4)	-8(3)	-16(4)
O(72)	46(3)	83(4)	73(3)	-2(3)	-12(2)	-6(3)
C(72)	79(5)	121(8)	74(5)	10(6)	-22(4)	-35(6)
C(73)	64(6)	214(14)	148(9)	-29(10)	-14(6)	-40(8)
N(1')	43(3)	46(4)	56(3)	0(3)	-3(3)	0(3)
C(2')	49(4)	61(5)	64(4)	-2(4)	-6(3)	-3(4)
C(3')	39(4)	50(4)	50(4)	3(4)	-4(3)	-2(3)
N(4')	42(3)	55(4)	55(3)	11(3)	-6(2)	-4(3)
C(5')	60(4)	61(5)	56(4)	21(4)	-10(3)	-22(4)
C(6')	60(5)	62(5)	45(4)	-6(4)	-2(3)	-6(4)
C(7')	44(4)	60(5)	54(4)	13(4)	-3(3)	-6(4)
C(7A')	42(4)	48(4)	64(4)	19(4)	-4(3)	-5(3)
C(8')	79(6)	94(8)	70(6)	28(6)	-27(5)	-35(6)
O(8')	98(5)	119(6)	121(5)	40(5)	-54(4)	-6(4)
O(9')	138(6)	144(7)	53(4)	11(5)	-33(4)	-41(5)
C(10')	134(9)	143(11)	72(7)	-15(7)	13(6)	-48(9)
C(11')	98(6)	97(7)	73(6)	-9(5)	11(5)	-32(6)
C'	63(4)	45(5)	82(5)	-5(4)	-11(4)	-6(4)
C(1B')	46(4)	59(5)	63(5)	-11(4)	3(4)	-18(4)
C(12')	52(4)	78(6)	69(5)	-20(5)	3(4)	5(4)
C(13')	51(4)	92(7)	83(5)	-2(6)	-8(4)	-3(5)
C(14')	61(5)	84(6)	67(5)	-11(5)	0(4)	-17(5)
C(15')	80(6)	79(6)	78(6)	-17(5)	6(5)	-21(5)
C(16')	62(5)	71(6)	92(6)	-23(5)	-2(4)	-8(4)
C(31')	43(4)	48(4)	54(4)	-4(4)	1(3)	7(3)
C(32')	50(4)	77(6)	61(5)	16(5)	0(4)	-1(4)
C(33')	70(5)	69(6)	66(5)	-1(4)	7(4)	-7(4)
C(34')	50(4)	68(5)	80(5)	-20(5)	15(4)	-8(4)
C(35')	47(4)	71(6)	78(5)	5(5)	3(4)	2(4)
C(36')	51(4)	60(5)	67(5)	-4(4)	-7(4)	3(4)
C(71')	56(5)	62(5)	54(4)	6(4)	0(4)	-6(4)
O(71')	60(3)	115(5)	105(4)	49(4)	-4(3)	11(3)
O(72')	51(3)	81(4)	90(4)	10(3)	-13(2)	-11(3)
C(72')	43(4)	129(8)	108(7)	25(7)	-14(4)	-34(5)
C(73')	66(6)	199(13)	119(8)	8(9)	2(5)	-38(8)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for JSPHNO.

	x	y	z	U(eq)
H(2A)	201(5)	-6409(7)	1203(4)	70
H(2B)	422(5)	-5834(7)	1934(4)	70
H(3A)	1235(5)	-4695(7)	718(3)	55
H(5A)	880(5)	-2493(7)	470(3)	62
H(6A)	-313(5)	-687(7)	650(3)	69

H(7A)	-1656(6)	-1789(7)	1522(3)	69
H(7AA)	-501(5)	-3248(7)	2084(3)	56
H(10A)	1174(7)	1073(9)	1136(4)	103
H(10B)	1455(7)	1066(9)	1908(4)	103
H(11A)	-458(6)	410(8)	1690(4)	90
H(11B)	247(6)	-768(8)	2054(4)	90
H(0A)	-2397(3)	-4654(5)	1829(2)	70
H(0B)	-1440(3)	-5316(5)	2306(2)	70
H(12A)	-2351(3)	-7447(5)	2567(2)	71
H(13A)	-3115(6)	-9536(8)	2264(4)	88
H(14A)	-3421(6)	-10066(9)	1146(4)	89
H(15A)	-2842(7)	-8516(9)	341(4)	90
H(16A)	-2087(6)	-6435(8)	646(4)	80
H(32A)	2618(5)	-3721(8)	2214(3)	79
H(33A)	4289(6)	-4657(8)	2705(4)	83
H(34A)	5098(6)	-6624(9)	2277(4)	96
H(35A)	4232(7)	-7628(10)	1353(5)	118
H(36A)	2562(6)	-6705(9)	880(4)	92
H(72A)	-3714(7)	-3023(11)	-137(4)	110
H(72B)	-3094(7)	-4441(11)	-12(4)	110
H(73A)	-5072(7)	-4652(15)	95(5)	213
H(73B)	-5056(7)	-3535(15)	660(5)	213
H(73C)	-4438(7)	-4950(15)	784(5)	213
H(2'A)	-1778(5)	553(7)	3449(3)	70
H(2'B)	-1003(5)	-617(7)	3783(3)	70
H(3'A)	-1258(5)	2107(7)	4263(3)	56
H(5'A)	-583(5)	2543(8)	5328(3)	71
H(6'A)	-2559(5)	2497(8)	5290(3)	67
H(7'A)	-2551(5)	-65(7)	5970(3)	63
H(7AB)	-1709(5)	-1141(7)	5119(3)	62
H(10C)	-1068(10)	3789(13)	6421(5)	139
H(10D)	-1548(10)	3289(13)	7112(5)	139
H(11C)	-2997(8)	3290(10)	6268(4)	108
H(11D)	-2834(8)	1844(10)	6601(4)	108
H'A	-3576(3)	-1712(5)	4497(2)	77
H'B	-2446(3)	-2182(5)	4121(2)	77
H(12B)	-4841(3)	100(5)	3729(2)	79
H(13B)	-5920(6)	59(9)	2738(4)	90
H(14B)	-5465(7)	-1432(9)	1896(4)	85
H(15B)	-3890(7)	-2887(9)	2036(4)	95
H(16B)	-2807(6)	-2870(8)	3020(4)	90
H(32B)	-62(6)	2592(8)	3230(4)	75
H(33B)	1793(6)	3022(8)	2834(4)	82
H(34B)	3421(6)	2236(8)	3427(4)	79
H(35B)	3189(6)	1037(8)	4415(4)	78
H(36B)	1316(5)	571(7)	4791(3)	71
H(72C)	-6141(6)	337(11)	5634(4)	112
H(72D)	-6059(6)	-1061(11)	5249(4)	112
H(73D)	-7175(7)	-1271(14)	6145(5)	192
H(73E)	-6125(7)	-785(14)	6608(5)	192
H(73F)	-6043(7)	-2181(14)	6224(5)	192