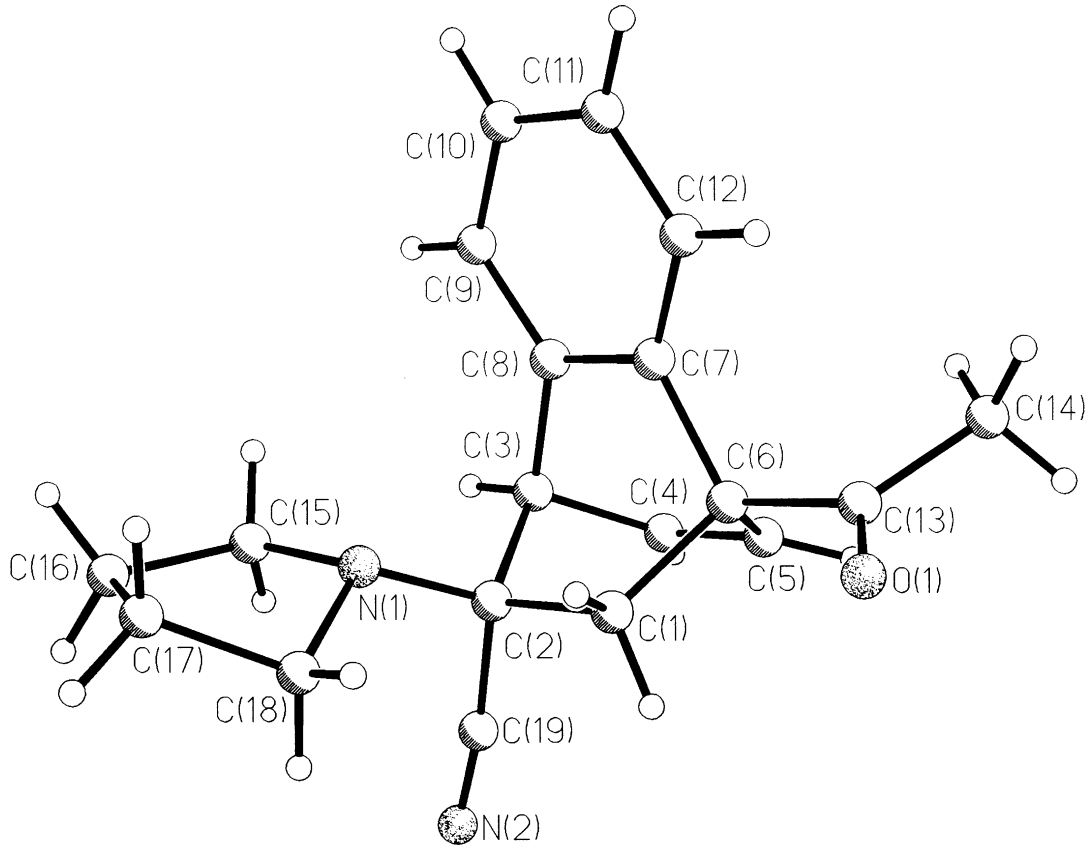
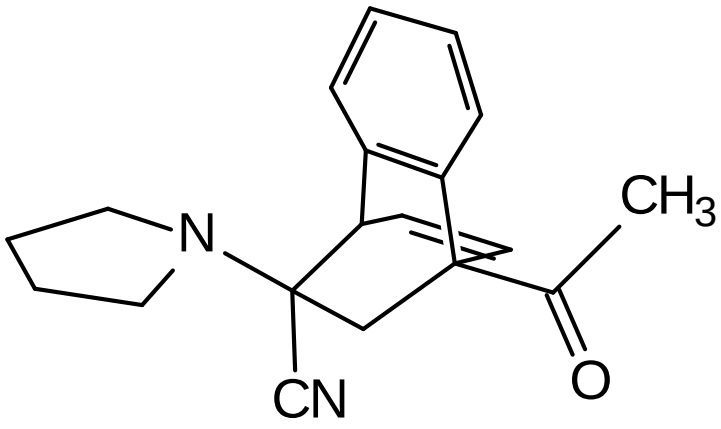
8. Anhang

8.1 Strukturparameter der kristallographisch untersuchten Verbindungen

8.1.1 Tabellen zur Röntgenstrukturanalyse von rel-(1R,4R,9R)-1-Acetyl-1,4-dihydro-9-pyrrolidinyl-1,4-ethanonaphthalin-9-carbonitril (3b)





Tab. 8.1.1.1: $C_{19}H_{20}N_2O$ (3b): Daten zur Kristallstrukturanalyse

Summenformel	$C_{19}H_{20}N_2O$
Formelgewicht	292.37
Kristallgröße [mm]	ca. 0.55•0.25•0.22
Messtemperatur [K]	150
Kristallsystem	monoklin
Raumgruppe	$P2_1/c$
a [Å]	9.910(2)
b [Å]	19.443(3)
c [Å]	8.557(2)
β [°]	112.80(1)
V [Å^3]	1519.9
Z	4
μ(MoKα) [mm^{-1}]	0.08
D_X [gcm^{-3}]	1.278
Messgerät	Siemens P4-Vierkreisdiffraktometer, (Drehanodengenerator, Graphitmonochromator, Szintillationszähler, λ = 0.71073 Å (MoKα))
Messmethode	ω-Scan
Absorptionskorrektur	empirisch (ψ-Scan)
Transmissionsbereich	0.944 - 0.910
Messbereich	4° < 2θ < 54° (+h,+k,±l)
Messgeschwindigkeit	intensitätsabhängig (4 bis 29 °min^{-1})
Strukturlösung	SHELXTL PLUS (direkte Methoden), H-Atome berechnet
Verfeinerung	Kleinste Quadrate (volle Matrix), alle Schweratome anisotrop, H-Atome berechnet (ein gemeinsamer isotroper Temperaturfaktor), ein Skalierungsfaktor, ein isotroper Extinktionsparameter
Symmetrieunabhängige Reflexe	3319, davon 2964 beobachtet (I>2•σ(I))
Zahl der Variablen	201
R-Indices [I>2•σ(I)]	R1 = 0.0387, wR2 = 0.1008
R-Indices (alle Reflexe)	R1 = 0.0436, wR2 = 0.1044
Rest-Differenzelektronendichten	0.335 and -0.247 e.Å^{-3}

Tab. 8.1.1.2: $C_{19}H_{20}N_2O$ (3b): Atomkoordinaten und ($x10^4$) und Koeffizienten der äquivalenten isotropen Temperaturfaktoren ($Å^2 x10^3$)[a]

	x	y	z	U(eq)
C(1)	3785(1)	8753(1)	863(1)	18(1)
C(2)	2244(1)	9040(1)	613(1)	17(1)
C(3)	2424(1)	9526(1)	2161(2)	19(1)
C(4)	3563(1)	10059(1)	2225(2)	22(1)
C(5)	4868(1)	9802(1)	2464(2)	21(1)
C(6)	4947(1)	9018(1)	2565(1)	17(1)
C(7)	4413(1)	8792(1)	3939(1)	18(1)
C(8)	3053(1)	9076(1)	3716(1)	19(1)
C(9)	2397(1)	8927(1)	4841(2)	23(1)
C(10)	3108(1)	8489(1)	6200(2)	26(1)
C(11)	4441(1)	8191(1)	6406(2)	25(1)
C(12)	5091(1)	8334(1)	5257(2)	21(1)
C(13)	6472(1)	8744(1)	2884(2)	21(1)
C(14)	7729(1)	9046(1)	4359(2)	27(1)
C(15)	-237(1)	8698(1)	397(2)	23(1)
C(16)	-1275(1)	8109(1)	-529(2)	29(1)
C(17)	-294(1)	7573(1)	-868(2)	27(1)
C(18)	952(1)	8006(1)	-944(2)	21(1)
C(19)	1652(1)	9473(1)	-962(2)	21(1)
N(1)	1227(1)	8481(1)	486(1)	17(1)
N(2)	1092(1)	9772(1)	-2203(2)	31(1)
O(1)	6653(1)	8305(1)	1982(1)	36(1)

Tab. 8.1.1.3: $C_{19}H_{20}N_2O$ (3b): Abstände [Å] und Winkel [°]

C(1)-C(6)	1.5538(15)	C(6)-C(1)-C(2)	109.83(9)
C(2)-C(1)	1.5614(15)	N(1)-C(2)-C(19)	109.42(9)

C(2)-N(1)	1.4581(14)	N(1)-C(2)-C(1)	110.76(9)
C(2)-C(19)	1.5023(16)	C(19)-C(2)-C(1)	110.16(9)
C(2)-C(3)	1.5799(16)	N(1)-C(2)-C(3)	111.00(9)
		C(19)-C(2)-C(3)	107.18(9)
		C(1)-C(2)-C(3)	108.25(9)
C(3)-C(8)	1.5104(16)	C(8)-C(3)-C(4)	108.47(9)
C(3)-C(4)	1.5175(17)	C(8)-C(3)-C(2)	105.41(9)
		C(4)-C(3)-C(2)	106.20(9)
C(4)-C(5)	1.3261(18)	C(5)-C(4)-C(3)	114.53(10)
C(5)-C(6)	1.5263(16)	C(4)-C(5)-C(6)	114.27(10)
C(6)-C(13)	1.5245(16)	C(13)-C(6)-C(5)	112.67(9)
C(6)-C(7)	1.5293(16)	C(13)-C(6)-C(7)	112.09(9)
		C(5)-C(6)-C(7)	107.79(9)
		C(13)-C(6)-C(1)	112.00(9)
		C(5)-C(6)-C(1)	106.00(9)
		C(7)-C(6)-C(1)	105.86(9)
C(7)-C(8)	1.3996(16)	C(12)-C(7)-C(8)	120.06(11)
		C(12)-C(7)-C(6)	127.34(10)
		C(8)-C(7)-C(6)	112.54(10)
C(8)-C(9)	1.3855(17)	C(9)-C(8)-C(7)	120.62(11)
		C(9)-C(8)-C(3)	126.04(11)
		C(7)-C(8)-C(3)	113.33(10)
C(9)-C(10)	1.3920(19)	C(8)-C(9)-C(10)	119.08(12)
C(10)-C(11)	1.3895(19)	C(11)-C(10)-C(9)	120.64(11)
C(11)-C(12)	1.3962(18)	C(10)-C(11)-C(12)	120.21(12)
C(12)-C(7)	1.3884(17)	C(7)-C(12)-C(11)	119.30(11)
C(13)-O(1)	1.2097(16)	O(1)-C(13)-C(14)	122.09(11)
C(13)-C(14)	1.5068(17)	O(1)-C(13)-C(6)	120.93(11)
		C(14)-C(13)-C(6)	116.97(10)
N(1)-C(15)	1.4842(15)	C(2)-N(1)-C(18)	115.51(9)
		C(2)-N(1)-C(15)	115.22(9)
		C(18)-N(1)-C(15)	105.85(9)
C(15)-C(16)	1.5385(18)	N(1)-C(15)-C(16)	105.05(10)
C(16)-C(17)	1.5267(19)	C(17)-C(16)-C(15)	104.99(10)
C(17)-C(18)	1.5161(17)	C(18)-C(17)-C(16)	102.60(10)
C(18)-N(1)	1.4721(15)	N(1)-C(18)-C(17)	101.82(9)
C(19)-N(2)	1.1468(17)	N(2)-C(19)-C(2)	174.13(13)

Tab. 8.1.1.4: $C_{19}H_{20}N_2O$ (3b): Koeffizienten der anisotropen Temperaturfaktoren ($Å^2 \times 10^3$)[a]

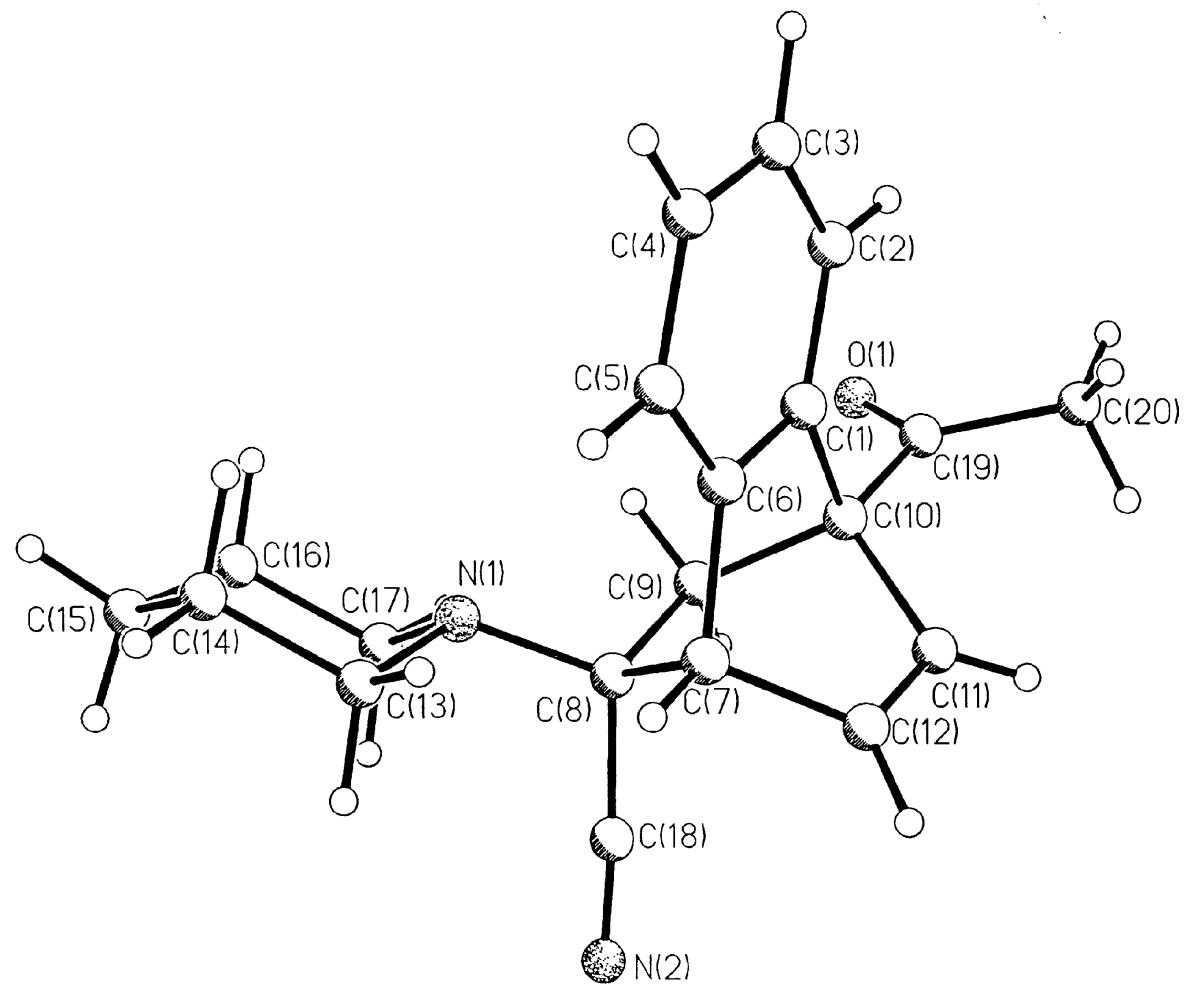
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	14(1)	20(1)	19(1)	-2(1)	6(1)	1(1)
C(2)	15(1)	18(1)	18(1)	0(1)	5(1)	1(1)
C(3)	16(1)	20(1)	22(1)	-3(1)	7(1)	3(1)
C(4)	24(1)	17(1)	24(1)	-2(1)	7(1)	0(1)
C(5)	21(1)	18(1)	22(1)	-2(1)	7(1)	-4(1)
C(6)	14(1)	18(1)	19(1)	-1(1)	6(1)	-1(1)
C(7)	15(1)	18(1)	18(1)	-4(1)	6(1)	-3(1)
C(8)	16(1)	19(1)	19(1)	-5(1)	6(1)	-2(1)
C(9)	19(1)	28(1)	23(1)	-9(1)	9(1)	-6(1)
C(10)	27(1)	31(1)	22(1)	-6(1)	12(1)	-12(1)
C(11)	28(1)	25(1)	20(1)	1(1)	5(1)	-7(1)
C(12)	19(1)	20(1)	22(1)	-1(1)	5(1)	-2(1)
C(13)	16(1)	25(1)	24(1)	2(1)	8(1)	1(1)
C(14)	14(1)	33(1)	31(1)	-1(1)	6(1)	-1(1)
C(15)	15(1)	28(1)	26(1)	-1(1)	8(1)	1(1)
C(16)	17(1)	40(1)	27(1)	-6(1)	8(1)	-6(1)
C(17)	23(1)	28(1)	28(1)	-4(1)	7(1)	-7(1)
C(18)	19(1)	23(1)	21(1)	-4(1)	7(1)	-2(1)
C(19)	19(1)	21(1)	24(1)	-1(1)	9(1)	1(1)
N(1)	14(1)	19(1)	19(1)	-2(1)	6(1)	-1(1)
N(2)	33(1)	31(1)	28(1)	7(1)	11(1)	6(1)
O(1)	21(1)	44(1)	39(1)	-13(1)	9(1)	7(1)

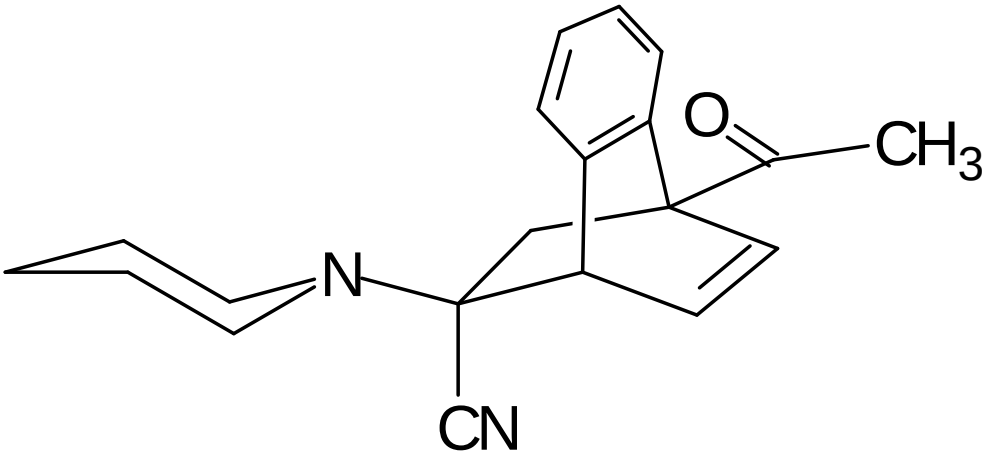
[a] Der anisotrope Temperaturfaktor ist definiert als
$\exp(-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*))$

Tab. 8.1.1.5: $C_{19}H_{20}N_2O$ (3b): Koordinaten der H-Atome ($x10^4$) und isotrope Temperaturfaktoren ($Å^2 x10^3$)

	x	y	z	U(eq)
H(1A)	4038	8899	-60	33(1)
H(1B)	3763	8259	865	33(1)
H(3A)	1512	9731	2058	33(1)
H(4A)	3353	10543	2096	33(1)
H(5A)	5692	10085	2572	33(1)
H(9A)	1463	9123	4680	33(1)
H(10A)	2677	8393	7006	33(1)
H(11A)	4920	7889	7344	33(1)
H(12A)	5991	8114	5370	33(1)
H(14C)	7356	9345	4991	33(1)
H(14A)	8357	9300	3953	33(1)
H(14B)	8293	8684	5081	33(1)
H(15A)	-227	8761	1514	33(1)
H(15B)	-530	9121	-220	33(1)
H(16A)	-2014	8269	-1570	33(1)
H(16B)	-1742	7918	168	33(1)
H(17A)	-802	7340	-1924	33(1)
H(17B)	50	7239	27	33(1)
H(18A)	670	8250	-1998	33(1)
H(18B)	1797	7728	-784	33(1)

8.1.2 Tabellen zur Röntgenstrukturanalyse von rel-(1R,4R,9R)-1-Acetyl-1,4-dihydro-9-pieperidinyl-1,4-ethanonaphthalin-9-carbonitril (3c)





Tab. 8.1.2.1: $C_{20}H_{22}N_2O$ (3c): Daten zur Kristallstrukturanalyse

Summenformel	$C_{20}H_{22}N_2O$
Formelgewicht	306.40
Kristallgröße [mm]	ca. 0.71•0.23•0.20
Messtemperatur [K]	150
Kristallsystem	orthorhombisch
Raumgruppe	$P2_12_12_1$
a [Å]	8.869(2)
b [Å]	10.552(2)
c [Å]	17.902(4)
V [$Å^3$]	1675.4
Z	4
μ(MoKα) [mm^{-1}]	0.08
D_X [gcm^{-3}]	1.215
Messgerät	Siemens P4-Vierkreisdiffraktometer, (Drehanodengenerator, Graphitmonochromator, Szintillationszähler, λ = 0.71073 Å (MoKα))
Messmethode	ω-Scan
Absorptionskorrektur	empirisch (ψ-Scan)
Transmissionsbereich	0.975 - 0.948
Messbereich	$4^o < 2\theta < 54^o$ (+h,+k,+l)
Messgeschwindigkeit	intensitätsabhängig (4 bis 29 $^o min^{-1}$)
Strukturlösung	SHELXTL PLUS (direkte Methoden), H-Atome berechnet
Verfeinerung	Kleinste Quadrate (volle Matrix), alle Schweratome anisotrop, H-Atome berechnet (ein gemeinsamer isotroper Temperaturfaktor), ein Skalierungsfaktor, ein isotroper Extinktionsparameter
Symmetrieunabhängige Reflexe	3659, davon 3342 beobachtet ($I>2\bullet\sigma(I)$)
Zahl der Variablen	210
R-Indices [$I>2\bullet\sigma(I)$]	R1 = 0.0362, wR2 = 0.0842
R-Indices (alle Reflexe)	R1 = 0.0425, wR2 = 0.0880
Rest-Differenzelektronendichten	0.227 and -0.163 e.$Å^{-3}$

Tab. 8.1.2.2: $C_{20}H_{22}N_2O$ (3c): Atomkoordinaten und ($x10^4$) und Koeffizienten der äquivalenten isotropen Temperaturfaktoren ($Å^2 x10^3$)[a]

	x	y	z	U(eq)
N(1)	1059(1)	9182(1)	1400(1)	19(1)
N(2)	-1092(2)	10948(2)	209(1)	37(1)
O(1)	-3724(1)	7515(1)	2554(1)	30(1)
C(1)	-1124(2)	9536(1)	3075(1)	18(1)
C(2)	-1049(2)	8891(1)	3753(1)	21(1)
C(3)	234(2)	9026(2)	4197(1)	25(1)
C(4)	1425(2)	9778(2)	3964(1)	23(1)
C(5)	1346(2)	10430(1)	3283(1)	20(1)
C(6)	61(2)	10313(1)	2846(1)	18(1)
C(7)	-219(2)	10968(1)	2105(1)	19(1)
C(8)	-361(2)	9888(1)	1501(1)	18(1)
C(9)	-1635(2)	8968(1)	1768(1)	20(1)
C(10)	-2400(2)	9480(1)	2494(1)	19(1)
C(11)	-2880(2)	10842(2)	2334(1)	23(1)
C(12)	-1757(2)	11593(2)	2133(1)	23(1)
C(13)	2393(2)	9981(2)	1269(1)	25(1)
C(14)	3805(2)	9172(2)	1285(1)	33(1)
C(15)	3773(2)	8124(2)	701(1)	31(1)
C(16)	2313(2)	7371(2)	777(1)	30(1)
C(17)	946(2)	8242(2)	790(1)	24(1)
C(18)	-817(2)	10505(2)	779(1)	24(1)
C(19)	-3656(2)	8608(2)	2765(1)	23(1)
C(20)	-4774(2)	9137(2)	3315(1)	32(1)

Tab. 8.1.2.3: $C_{20}H_{22}N_2O$ (3c): Abstände [Å] und Winkel [°]

C(1)-C(2)	1.392(2)	C(2)-C(1)-C(6)	120.48(14)
C(1)-C(6)	1.395(2)	C(2)-C(1)-C(10)	127.30(13)
C(1)-C(10)	1.539(2)	C(6)-C(1)-C(10)	112.20(12)
C(2)-C(3)	1.396(2)	C(1)-C(2)-C(3)	119.07(14)
C(3)-C(4)	1.385(2)	C(4)-C(3)-C(2)	120.54(14)
C(4)-C(5)	1.401(2)	C(3)-C(4)-C(5)	120.35(14)

C(5)-C(6)	1.387(2)	C(6)-C(5)-C(4)	119.21(14)
C(6)-C(7)	1.5164(19)	C(5)-C(6)-C(1)	120.34(13)
		C(5)-C(6)-C(7)	125.99(13)
		C(1)-C(6)-C(7)	113.67(12)
C(7)-C(8)	1.577(2)	C(12)-C(7)-C(6)	108.44(12)
		C(12)-C(7)-C(8)	105.41(12)
		C(6)-C(7)-C(8)	106.50(11)
C(8)-C(18)	1.503(2)	N(1)-C(8)-C(18)	110.10(12)
C(8)-C(9)	1.565(2)	N(1)-C(8)-C(9)	109.95(11)
		C(18)-C(8)-C(9)	109.72(12)
		N(1)-C(8)-C(7)	112.43(12)
		C(18)-C(8)-C(7)	107.34(11)
		C(9)-C(8)-C(7)	107.21(11)
C(9)-C(10)	1.562(2)	C(10)-C(9)-C(8)	110.73(12)
C(10)-C(19)	1.524(2)	C(19)-C(10)-C(11)	115.13(12)
C(10)-C(11)	1.526(2)	C(19)-C(10)-C(1)	110.15(12)
		C(11)-C(10)-C(1)	107.22(11)
		C(19)-C(10)-C(9)	111.95(12)
		C(11)-C(10)-C(9)	106.90(12)
		C(1)-C(10)-C(9)	104.89(11)
C(11)-C(12)	1.323(2)	C(12)-C(11)-C(10)	113.89(13)
C(12)-C(7)	1.516(2)	C(11)-C(12)-C(7)	115.23(13)
C(13)-C(14)	1.517(2)	N(1)-C(13)-C(14)	109.76(13)
C(14)-C(15)	1.521(2)	C(13)-C(14)-C(15)	112.40(14)
C(15)-C(16)	1.525(3)	C(14)-C(15)-C(16)	109.51(14)
C(16)-C(17)	1.521(2)	C(17)-C(16)-C(15)	111.29(13)
C(17)-N(1)	1.479(2)	N(1)-C(17)-C(16)	111.25(13)
N(1)-C(13)	1.472(2)	C(13)-N(1)-C(8)	114.59(11)
N(1)-C(8)	1.4744(19)	C(13)-N(1)-C(17)	108.79(11)
		C(8)-N(1)-C(17)	111.82(12)
C(18)-N(2)	1.147(2)	N(2)-C(18)-C(8)	176.03(17)
C(19)-C(20)	1.505(2)	O(1)-C(19)-C(20)	121.51(15)
C(19)-O(1)	1.2148(19)	O(1)-C(19)-C(10)	120.72(14)
		C(20)-C(19)-C(10)	117.75(14)

Tab. 8.1.2.4: $C_{20}H_{22}N_2O$ (3c): Koeffizienten der anisotropen Temperaturfaktoren ($Å^2 \times 10^3$)[a]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	23(1)	18(1)	17(1)	-4(1)	3(1)	0(1)
N(2)	53(1)	35(1)	23(1)	2(1)	-6(1)	3(1)
O(1)	25(1)	25(1)	40(1)	-1(1)	6(1)	-4(1)
C(1)	20(1)	16(1)	18(1)	-3(1)	1(1)	5(1)
C(2)	24(1)	20(1)	20(1)	0(1)	3(1)	2(1)
C(3)	34(1)	24(1)	17(1)	-1(1)	0(1)	7(1)
C(4)	24(1)	25(1)	21(1)	-6(1)	-4(1)	7(1)
C(5)	22(1)	17(1)	21(1)	-6(1)	2(1)	3(1)
C(6)	23(1)	13(1)	17(1)	-4(1)	2(1)	3(1)
C(7)	26(1)	15(1)	16(1)	-2(1)	2(1)	-1(1)
C(8)	23(1)	17(1)	15(1)	-1(1)	0(1)	0(1)
C(9)	23(1)	19(1)	19(1)	-2(1)	1(1)	0(1)
C(10)	19(1)	20(1)	18(1)	-1(1)	0(1)	2(1)
C(11)	25(1)	24(1)	20(1)	-1(1)	-1(1)	10(1)
C(12)	32(1)	18(1)	18(1)	-1(1)	-2(1)	7(1)
C(13)	26(1)	24(1)	25(1)	-6(1)	4(1)	-3(1)
C(14)	24(1)	41(1)	35(1)	-7(1)	0(1)	2(1)
C(15)	34(1)	34(1)	26(1)	-2(1)	8(1)	11(1)
C(16)	45(1)	22(1)	22(1)	-2(1)	11(1)	5(1)
C(17)	31(1)	22(1)	20(1)	-5(1)	5(1)	-3(1)
C(18)	29(1)	21(1)	23(1)	-2(1)	-2(1)	0(1)
C(19)	18(1)	29(1)	22(1)	2(1)	-1(1)	1(1)
C(20)	23(1)	43(1)	30(1)	-5(1)	7(1)	1(1)

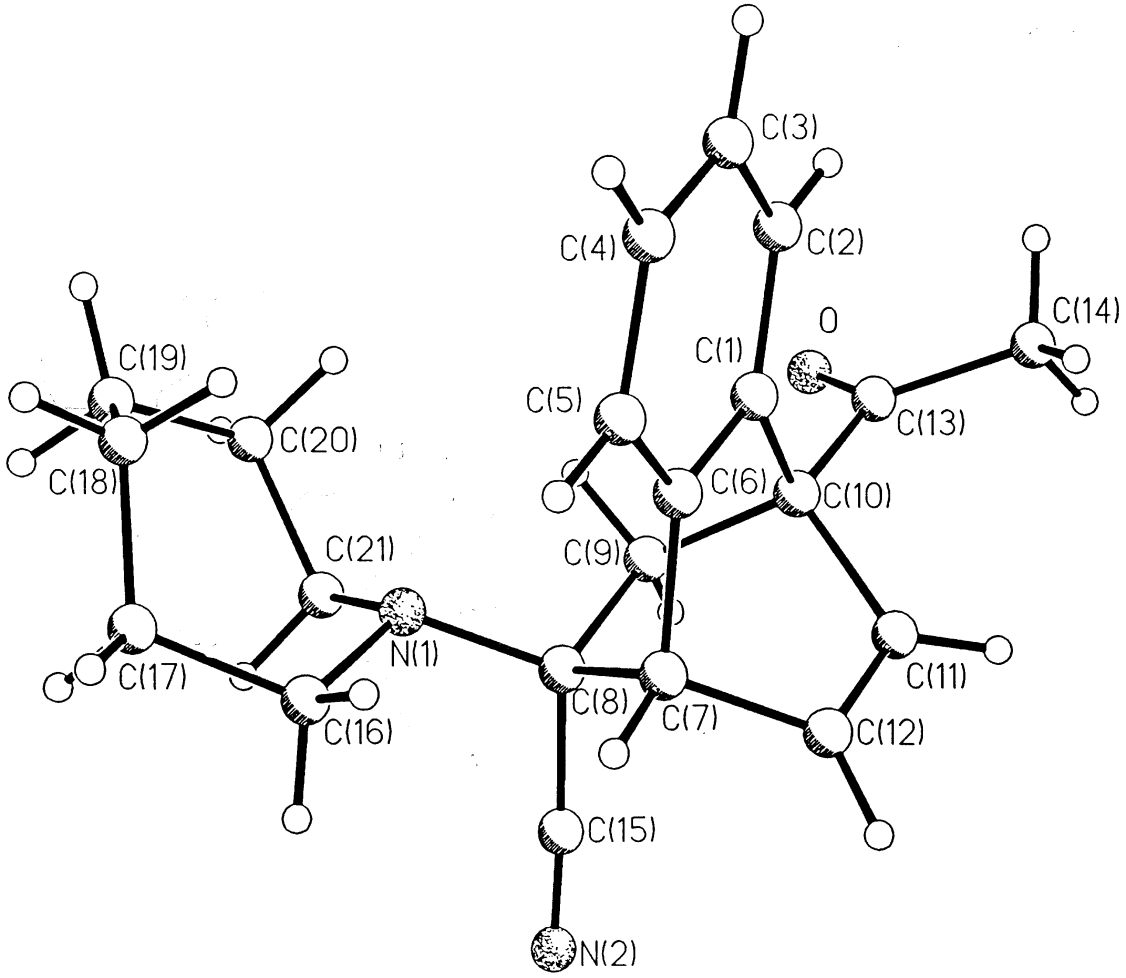
[a] Der anisotrope Temperaturfaktor ist definiert als

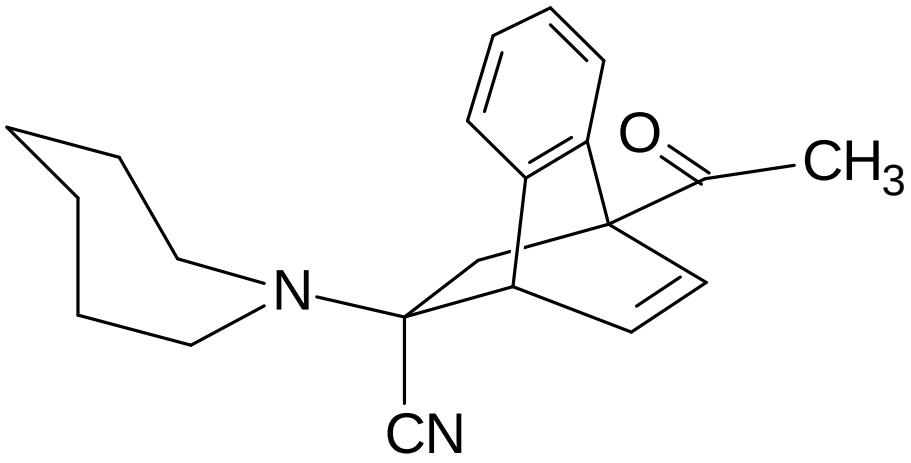
$$\exp(-2\pi^2(U_{11}h^2a^{*2}+U_{22}k^2b^{*2}+U_{33}l^2c^{*2}+2U_{12}hka^*b^*+2U_{13}hla^*c^*+2U_{23}klb^*c^*)$$

Tab.8.1.2.5: $C_{20}H_{22}N_2O$(3c): Koordinaten der H-Atome ($x10^4$) und isotrope Temperaturfaktoren ($Å^2 x10^3$)

	x	y	z	U(eq)
H(2A)	-1867	8360	3911	31(1)
H(3A)	291	8595	4668	31(1)
H(4A)	2309	9851	4270	31(1)
H(5A)	2171	10952	3123	31(1)
H(7A)	564	11563	1985	31(1)
H(9A)	-1213	8146	1863	31(1)
H(9B)	-2378	8883	1381	31(1)
H(11A)	-3904	11128	2376	31(1)
H(12A)	-1907	12470	2014	31(1)
H(13A)	2453	10623	1648	31(1)
H(13B)	2307	10394	793	31(1)
H(14A)	3911	8800	1771	31(1)
H(14B)	4668	9701	1198	31(1)
H(15A)	4621	7571	770	31(1)
H(15B)	3838	8486	210	31(1)
H(16A)	2340	6883	1229	31(1)
H(16B)	2227	6793	365	31(1)
H(17A)	869	8676	320	31(1)
H(17B)	49	7745	855	31(1)
H(20C)	-4263	9655	3676	31(1)
H(20A)	-5285	8453	3561	31(1)
H(20B)	-5514	9631	3053	31(1)

7.1.3 Tabellen zur Röntgenstrukturanalyse von rel-(1R,4R,9R)-1-Acetyl-1,4-dihydro-9-hexamethylenimino-1,4-ethanonaphthalin-9-carbonitril (3d)





Tab. 8.1.3.1: $C_{21}H_{24}N_2O$ (3d): Daten zur Kristallstrukturanalyse

Summenformel	$C_{21}H_{24}N_2O$
Formelgewicht	320.42
Kristallgröße [mm]	ca. 0.59•0.22•0.22
Messtemperatur [K]	150
Kristallsystem	monoklin
Raumgruppe	$P2_1/c$
a [Å]	13.362(4)
b [Å]	9.718(2)
c [Å]	13.757(4)
β [°]	99.72(2)
V [Å^3]	760.7
Z	4
μ(MoKα) [mm^{-1}]	0.07
D_X [gcm^{-3}]	1.209
Messgerät	Siemens P4-Vierkreisdiffraktometer, (Drehanodengenerator, Graphitmonochromator, Szintillationszähler, λ = 0.71073 Å (MoKα))
Messmethode	ω-Scan
Absorptionskorrektur	empirisch (ψ-Scan)
Transmissionsbereich	0.973 - 0.965
Messbereich	4° < 2θ < 54° (±h,+k,+l)
Messgeschwindigkeit	intensitätsabhängig (4 bis 29 °min^{-1})
Strukturlösung	SHELXTL PLUS (direkte Methoden), H-Atome berechnet
Verfeinerung	Kleinste Quadrate (volle Matrix), alle Schweratome anisotrop, H-Atome berechnet (ein gemeinsamer isotroper Temperaturfaktor), ein Skalierungsfaktor, ein isotroper Extinktionsparameter
Symmetrieunabhängige Reflexe	3860, davon 2987 beobachtet (I>2•σ(I))
Zahl der Variablen	219
R-Indices [I>2•σ(I)]	R1 = 0.0472, wR2 = 0.1096
R-Indices (alle Reflexe)	R1 = 0.0665, wR2 = 0.1200
Rest-Differenzelektronendichten	0.280 and -0.234 e.Å^{-3}

Tab. 8.1.3.2: $C_{21}H_{24}N_2O$ (3d): Atomkoordinaten und ($x10^4$) und Koeffizienten der äquivalenten isotropen Temperaturfaktoren ($Å^2 x10^3$)[a]

_	x	y	z	U(eq)
C(1)	1794(1)	-63(2)	-11(1)	19(1)
C(2)	2021(1)	-1450(2)	116(1)	24(1)
C(3)	2307(1)	-1969(2)	1065(1)	28(1)
C(4)	2382(1)	-1108(2)	1874(1)	29(1)
C(5)	2183(1)	293(2)	1744(1)	26(1)
C(6)	1880(1)	813(2)	803(1)	21(1)
C(7)	1609(1)	2298(2)	536(1)	23(1)
C(8)	2395(1)	2795(2)	-126(1)	24(1)
C(9)	2299(1)	1800(2)	-1030(1)	25(1)
C(10)	1463(1)	702(2)	-984(1)	22(1)
C(11)	494(1)	1476(2)	-893(1)	26(1)
C(12)	578(1)	2312(2)	-123(1)	26(1)
C(13)	1350(1)	-232(2)	-1887(1)	29(1)
C(14)	470(1)	-1217(2)	-2052(1)	40(1)
C(15)	2080(1)	4218(2)	-484(1)	32(1)
C(16)	3578(1)	3546(2)	1350(1)	36(1)
C(17)	4659(2)	3460(2)	1918(1)	43(1)
C(18)	5195(2)	2097(2)	1817(2)	44(1)
C(19)	5734(2)	2057(3)	933(2)	56(1)
C(20)	5054(2)	2087(3)	-78(2)	50(1)
C(21)	4207(1)	3143(2)	-200(1)	38(1)
N(1)	3435(1)	2793(1)	411(1)	26(1)
N(2)	1884(2)	5313(2)	-752(1)	47(1)
O	1945(1)	-174(2)	-2454(1)	55(1)

Tab. 8.1.3.3: $C_{21}H_{24}N_2O$ (3d): Abstände [Å] und Winkel [°]

C(1)-C(2)	1.387(2)	C(2)-C(1)-C(6)	120.33(14)
C(1)-C(6)	1.396(2)	C(2)-C(1)-C(10)	127.38(13)
C(1)-C(10)	1.529(2)	C(6)-C(1)-C(10)	112.27(13)
C(2)-C(3)	1.392(2)	C(1)-C(2)-C(3)	119.33(14)

C(3)-C(4)	1.382(2)	C(4)-C(3)-C(2)	120.45(15)
C(4)-C(5)	1.393(2)	C(3)-C(4)-C(5)	120.17(15)
C(5)-C(6)	1.384(2)	C(6)-C(5)-C(4)	119.73(14)
C(6)-C(7)	1.518(2)	C(5)-C(6)-C(1)	119.95(14)
		C(5)-C(6)-C(7)	126.39(13)
		C(1)-C(6)-C(7)	113.65(13)
C(7)-C(8)	1.577(2)	C(12)-C(7)-C(6)	107.95(12)
		C(12)-C(7)-C(8)	106.15(12)
		C(6)-C(7)-C(8)	106.07(12)
C(8)-N(1)	1.460(2)	N(1)-C(8)-C(15)	110.89(13)
C(8)-C(15)	1.504(2)	N(1)-C(8)-C(9)	110.20(12)
C(8)-C(9)	1.563(2)	C(15)-C(8)-C(9)	109.08(13)
		N(1)-C(8)-C(7)	112.12(12)
		C(15)-C(8)-C(7)	107.11(13)
		C(9)-C(8)-C(7)	107.30(12)
C(9)-C(10)	1.554(2)	C(10)-C(9)-C(8)	110.79(12)
C(10)-C(11)	1.522(2)	C(11)-C(10)-C(13)	113.07(13)
C(10)-C(13)	1.525(2)	C(11)-C(10)-C(1)	107.01(12)
		C(13)-C(10)-C(1)	113.46(13)
		C(11)-C(10)-C(9)	106.95(12)
		C(13)-C(10)-C(9)	110.42(12)
		C(1)-C(10)-C(9)	105.44(12)
C(11)-C(12)	1.325(2)	C(12)-C(11)-C(10)	114.22(14)
C(12)-C(7)	1.517(2)	C(11)-C(12)-C(7)	114.75(14)
C(13)-O	1.206(2)	O-C(13)-C(14)	121.05(15)
C(13)-C(14)	1.503(2)	O-C(13)-C(10)	120.89(15)
		C(14)-C(13)-C(10)	118.06(13)
C(15)-N(2)	1.141(2)	N(2)-C(15)-C(8)	177.1(2)
N(1)-C(16)	1.468(2)	C(8)-N(1)-C(16)	114.57(13)
		C(8)-N(1)-C(21)	114.12(13)
		C(16)-N(1)-C(21)	112.77(13)
C(16)-C(17)	1.524(3)	N(1)-C(16)-C(17)	113.22(15)
C(17)-C(18)	1.523(3)	C(18)-C(17)-C(16)	114.86(15)
C(18)-C(19)	1.516(3)	C(19)-C(18)-C(17)	112.94(18)
C(19)-C(20)	1.528(3)	C(18)-C(19)-C(20)	116.04(17)
C(20)-C(21)	1.515(3)	C(21)-C(20)-C(19)	115.61(17)
C(21)-N(1)	1.477(2)	N(1)-C(21)-C(20)	111.21(16)

Tab. 8.1.3.4: $C_{21}H_{24}N_2O$ (3d): Koeffizienten der anisotropen Temperaturfaktoren ($Å^2 \times 10^3$)[a]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	19(1)	19(1)	20(1)	-1(1)	5(1)	-2(1)
C(2)	23(1)	19(1)	30(1)	-3(1)	8(1)	-1(1)
C(3)	28(1)	21(1)	37(1)	6(1)	9(1)	4(1)
C(4)	30(1)	29(1)	28(1)	8(1)	2(1)	2(1)
C(5)	29(1)	26(1)	22(1)	-1(1)	5(1)	-1(1)
C(6)	22(1)	17(1)	24(1)	0(1)	7(1)	-1(1)
C(7)	32(1)	17(1)	22(1)	-2(1)	9(1)	1(1)
C(8)	33(1)	17(1)	24(1)	-1(1)	8(1)	-4(1)
C(9)	34(1)	20(1)	22(1)	-2(1)	8(1)	-7(1)
C(10)	27(1)	19(1)	20(1)	-1(1)	5(1)	-4(1)
C(11)	27(1)	25(1)	25(1)	8(1)	2(1)	1(1)
C(12)	29(1)	20(1)	30(1)	5(1)	8(1)	5(1)
C(13)	37(1)	27(1)	23(1)	-3(1)	7(1)	-8(1)
C(14)	41(1)	43(1)	36(1)	-16(1)	8(1)	-15(1)
C(15)	47(1)	22(1)	26(1)	-2(1)	10(1)	-5(1)
C(16)	44(1)	34(1)	30(1)	-11(1)	5(1)	-4(1)
C(17)	51(1)	45(1)	31(1)	-10(1)	3(1)	-13(1)
C(18)	34(1)	49(1)	46(1)	-1(1)	-2(1)	-8(1)
C(19)	31(1)	77(2)	58(1)	-16(1)	6(1)	-8(1)
C(20)	30(1)	77(2)	46(1)	-20(1)	13(1)	-13(1)
C(21)	43(1)	40(1)	34(1)	-9(1)	14(1)	-23(1)
N(1)	31(1)	23(1)	25(1)	-5(1)	8(1)	-8(1)
N(2)	82(1)	22(1)	39(1)	1(1)	12(1)	-1(1)
O	72(1)	59(1)	44(1)	-28(1)	36(1)	-35(1)

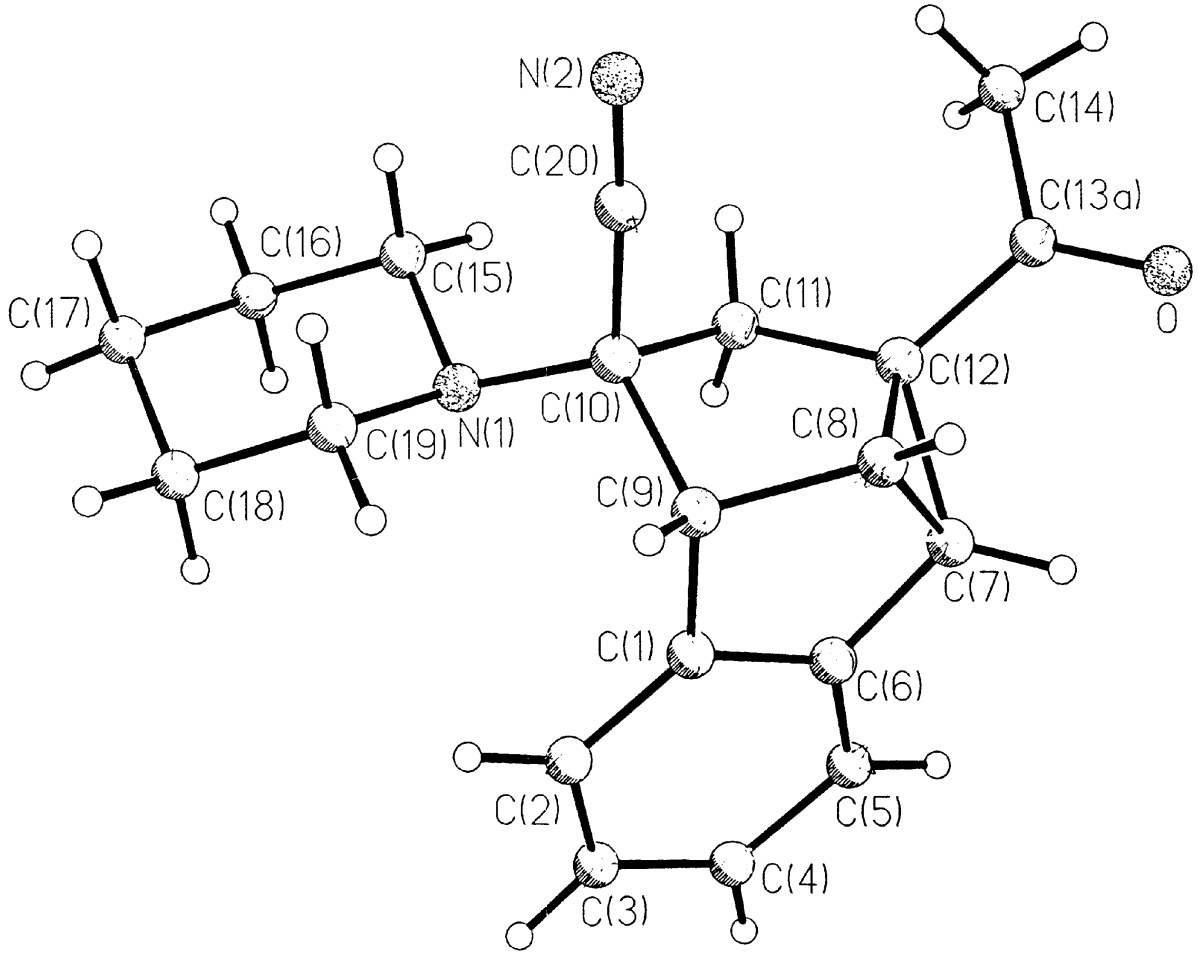
[a] Der anisotrope Temperaturfaktor ist definiert als

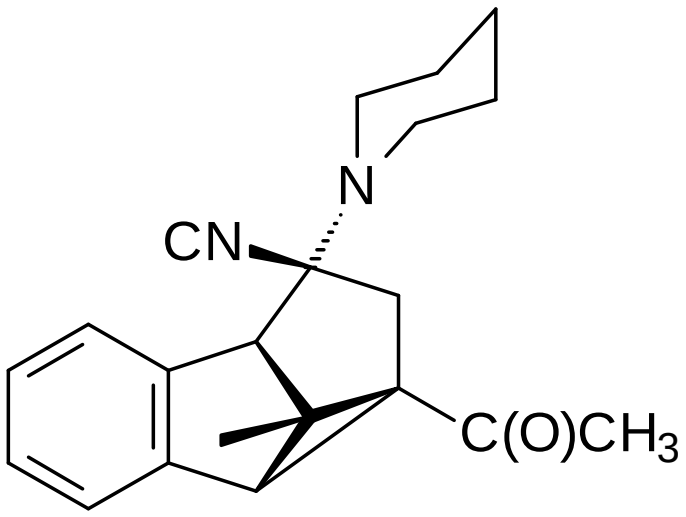
$$\exp(-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*)$$

Tab. 8.1.3.5: $C_{21}H_{24}N_2O$ (3d): Koordinaten der H-Atome ($x10^4$) und isotrope Temperaturfaktoren ($Å^2 x10^3$)

	x	y	z	U(eq)
H(2)	1994	-2038	-449	45(1)
H(3)	2440	-2936	1156	45(1)
H(4)	2567	-1476	2527	45(1)
H(5)	2261	901	2302	45(1)
H(7)	1627	2865	1111	45(1)
H(9A)	2141	2318	-1631	45(1)
H(9B)	2938	1345	-1027	45(1)
H(11)	-127	1362	-1352	45(1)
H(12)	32	2889	6	45(1)
H(14A)	725	-2136	-2088	45(1)
H(14B)	57	-1011	-2676	45(1)
H(14C)	78	-1145	-1530	45(1)
H(16A)	3396	4493	1221	45(1)
H(16B)	3125	3172	1755	45(1)
H(17A)	4649	3635	2603	45(1)
H(17B)	5049	4178	1682	45(1)
H(18A)	4700	1372	1755	45(1)
H(18B)	5675	1935	2408	45(1)
H(19A)	6136	1234	973	45(1)
H(19B)	6190	2826	974	45(1)
H(20A)	4750	1195	-201	45(1)
H(20B)	5466	2250	-574	45(1)
H(21A)	3891	3188	-880	45(1)
H(21B)	4488	4031	-10	45(1)

8.1.4. Tabellen zur Röntgenstrukturanalyse von *rel*-(2*R*,3*S*,4*S*,6*S*,7*S*)-4-Acetyl-6-piperidinyl-tetracyclo-[6.4.0.0$^{2.4}$.0$^{3.7}$]-dodeca-8,10,12-trien-6-carbonitril (7c)





Tab. 8.1.4.1: $C_{20}H_{22}N_2O$ (7c): Daten zur Kristallstrukturanalyse

Summenformel	$C_{20}H_{22}N_2O$
Formelgewicht	306.40
Kristallgröße [mm]	ca. 0.62•0.27•0.25
Messtemperatur [K]	150
Kristallsystem	monoklin
Raumgruppe	$P2_1/c$
a [Å]	16.764(3)
b [Å]	9.432(1)
c [Å]	10.497(2))
β [°]	103.25(1)
V [Å^3]	1615.56
Z	4
μ(MoKα) [mm^{-1}]	0.08
D_X [gcm^{-3}]	1.260
Messgerät	Siemens P4-Vierkreisdiffraktometer, (Drehanodengenerator, Graphitmonochromator, Szintillationszähler, λ= 0.71073 Å (MoKα))
Messmethode	ω-Scan
Absorptionskorrektur	empirisch (ψ-Scan)
Transmissionsbereich	0.949 - 0.922
Messbereich	$4° < 2\theta < 54°$ (±h,+k,+l)
Messgeschwindigkeit	intensitätsabhängig (4 bis 29 °min^{-1})
Strukturlösung	SHELXTL PLUS (direkte Methoden), H-Atome berechnet
Verfeinerung	Kleinste Quadrate (volle Matrix), alle Schweratome anisotrop, H-Atome berechnet (ein gemeinsamer isotroper Temperaturfaktor), ein Skalierungsfaktor, ein isotroper Extinktionsparameter
Symmetrieunabhängige Reflexe	3521, davon 3017 beobachtet (I>2•σ(I))
Zahl der Variablen	210
R-Indices [I>2•σ(I)]	R1 = 0.0398, wR2 = 0.0996
R-Indices (alle Reflexe)	R1 = 0.0477, wR2 = 0.1054
Rest-Differenzelektronendichten	0.306 and -0.262 e.Å^{-3}

Tab. 8.1.4.2. $C_{20}H_{22}N_2O$ (7c): Atomkoordinaten und ($x10^4$) und Koeffizienten der äquivalenten isotropen Temperaturfaktoren ($Å^2 x10^3$)[a]

	x	y	z	U(eq)
C(1)	8509(1)	19(1)	8178(1)	16(1)
C(2)	8458(1)	-392(1)	9427(1)	19(1)
C(3)	9048(1)	-1323(1)	10122(1)	23(1)
C(4)	9664(1)	-1855(1)	9569(1)	23(1)
C(5)	9708(1)	-1460(1)	8308(1)	21(1)
C(6)	9134(1)	-506(1)	7627(1)	17(1)
C(7)	9082(1)	139(1)	6321(1)	18(1)
C(8)	8423(1)	1245(1)	6136(1)	17(1)
C(9)	7947(1)	984(1)	7206(1)	15(1)
C(10)	7189(1)	100(1)	6458(1)	14(1)
C(11)	7591(1)	-945(1)	5644(1)	15(1)
C(12)	8271(1)	-82(1)	5271(1)	16(1)
C(13)	8345(1)	90(1)	3893(1)	19(1)
C(14)	7748(1)	-684(2)	2837(1)	35(1)
C(15)	6074(1)	-1525(1)	6557(1)	18(1)
C(16)	5661(1)	-2353(1)	7473(1)	20(1)
C(17)	5320(1)	-1364(1)	8366(1)	23(1)
C(18)	5992(1)	-359(1)	9064(1)	22(1)
C(19)	6379(1)	421(1)	8090(1)	18(1)
C(20)	6649(1)	1082(1)	5502(1)	18(1)
N(1)	6728(1)	-598(1)	7297(1)	14(1)
N(2)	6207(1)	1786(1)	4782(1)	30(1)
O	8866(1)	861(1)	3626(1)	30(1)

Tab. 8.1.4.3: $C_{20}H_{22}N_2O$ (7c): Abstände [Å] und Winkel [°]

C(1)-C(2)	1.3885(17)	C(2)-C(1)-C(6)	120.41(11)
C(1)-C(6)	1.3977(17)	C(2)-C(1)-C(9)	129.52(11)
C(1)-C(9)	1.5219(16)	C(6)-C(1)-C(9)	110.05(10)
C(2)-C(3)	1.3977(17)	C(1)-C(2)-C(3)	118.62(11)
C(3)-C(4)	1.3899(19)	C(4)-C(3)-C(2)	120.90(11)
C(4)-C(5)	1.3929(18)	C(3)-C(4)-C(5)	120.45(12)
C(5)-C(6)	1.3899(17)	C(6)-C(5)-C(4)	118.73(11)

C(6)-C(7)	1.4847(16)	C(5)-C(6)-C(1)	120.86(11)
		C(5)-C(6)-C(7)	128.87(11)
		C(1)-C(6)-C(7)	110.23(10)
C(7)-C(8)	1.4989(16)	C(6)-C(7)-C(8)	106.87(10)
C(7)-C(12)	1.5555(16)	C(6)-C(7)-C(12)	117.10(10)
		C(8)-C(7)-C(12)	60.21(7)
C(8)-C(12)	1.5329(16)	C(7)-C(8)-C(12)	61.73(8)
C(8)-C(9)	1.5405(15)	C(7)-C(8)-C(9)	106.52(9)
		C(12)-C(8)-C(9)	104.91(9)
C(9)-C(10)	1.5705(15)	C(1)-C(9)-C(8)	103.82(9)
		C(1)-C(9)-C(10)	108.90(9)
		C(8)-C(9)-C(10)	102.45(9)
C(10)-N(1)	1.4553(14)	N(1)-C(10)-C(20)	111.07(9)
C(10)-C(20)	1.5059(16)	N(1)-C(10)-C(11)	113.77(9)
C(10)-C(11)	1.5556(15)	C(20)-C(10)-C(11)	107.07(9)
		N(1)-C(10)-C(9)	114.73(9)
		C(20)-C(10)-C(9)	107.50(9)
		C(11)-C(10)-C(9)	102.02(9)
C(11)-C(12)	1.5227(15)	C(12)-C(11)-C(10)	104.29(9)
C(12)-C(13)	1.4896(16)	C(13)-C(12)-C(11)	122.82(10)
		C(13)-C(12)-C(8)	116.52(10)
		C(11)-C(12)-C(8)	108.48(9)
		C(13)-C(12)-C(7)	114.81(10)
		C(11)-C(12)-C(7)	118.29(10)
		C(8)-C(12)-C(7)	58.06(7)
C(13)-O	1.2173(15)	O-C(13)-C(12)	120.84(11)
C(13)-C(14)	1.5013(18)	O-C(13)-C(14)	120.85(11)
		C(12)-C(13)-C(14)	118.29(11)
N(1)-C(15)	1.4763(14)	C(10)-N(1)-C(19)	112.36(9)
		C(10)-N(1)-C(15)	112.49(9)
		C(19)-N(1)-C(15)	109.91(9)
C(15)-C(16)	1.5233(16)	N(1)-C(15)-C(16)	111.19(10)
C(16)-C(17)	1.5247(17)	C(15)-C(16)-C(17)	111.33(10)
C(17)-C(18)	1.5251(18)	C(16)-C(17)-C(18)	109.58(10)
C(18)-C(19)	1.5212(16)	C(19)-C(18)-C(17)	111.10(10)
C(19)-N(1)	1.4762(15)	N(1)-C(19)-C(18)	110.44(10)
C(20)-N(2)	1.1429(16)	N(2)-C(20)-C(10)	176.63(13)

Tab. 8.1.4.4: $C_{20}H_{22}N_2O$ (7c): Koeffizienten der anisotropen Temperaturfaktoren ($Å^2 \times 10^3$)[a]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	14(1)	16(1)	17(1)	-2(1)	1(1)	-3(1)
C(2)	18(1)	23(1)	17(1)	-1(1)	4(1)	-2(1)
C(3)	23(1)	26(1)	17(1)	4(1)	1(1)	-4(1)
C(4)	19(1)	23(1)	24(1)	3(1)	-2(1)	0(1)
C(5)	15(1)	23(1)	24(1)	0(1)	3(1)	1(1)
C(6)	14(1)	20(1)	16(1)	-1(1)	2(1)	-3(1)
C(7)	14(1)	21(1)	18(1)	0(1)	4(1)	-2(1)
C(8)	16(1)	16(1)	18(1)	0(1)	4(1)	-3(1)
C(9)	15(1)	14(1)	16(1)	-1(1)	4(1)	-2(1)
C(10)	14(1)	14(1)	15(1)	1(1)	3(1)	1(1)
C(11)	15(1)	16(1)	15(1)	-2(1)	5(1)	-2(1)
C(12)	14(1)	17(1)	16(1)	0(1)	4(1)	-2(1)
C(13)	19(1)	21(1)	19(1)	2(1)	7(1)	3(1)
C(14)	42(1)	47(1)	17(1)	-4(1)	10(1)	-18(1)
C(15)	16(1)	20(1)	19(1)	-2(1)	4(1)	-3(1)
C(16)	17(1)	20(1)	26(1)	2(1)	7(1)	-3(1)
C(17)	20(1)	25(1)	27(1)	4(1)	12(1)	0(1)
C(18)	25(1)	23(1)	22(1)	0(1)	12(1)	1(1)
C(19)	19(1)	16(1)	21(1)	-1(1)	9(1)	2(1)
C(20)	17(1)	18(1)	19(1)	1(1)	6(1)	-2(1)
N(1)	14(1)	14(1)	17(1)	-1(1)	6(1)	-1(1)
N(2)	26(1)	31(1)	32(1)	13(1)	3(1)	4(1)
O	29(1)	41(1)	23(1)	4(1)	10(1)	-12(1)

[a] Der anisotrope Temperaturfaktor ist definiert als

$$\exp(-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*)$$

Tab. 8.1.4.5: $C_{20}H_{22}N_2O$ (7c): Koordinaten der H-Atome ($x10^4$) und isotrope Temperaturfaktoren ($Å^2 x10^3$)

	x	y	z	U(eq)
H(2A)	8023	-46	9800	26(1)
H(3A)	9029	-1595	10996	26(1)
H(4A)	10065	-2492	10063	26(1)
H(5A)	10123	-1841	7910	26(1)
H(7A)	9579	334	6045	26(1)
H(8A)	8486	2172	5794	26(1)
H(9A)	7799	1836	7595	26(1)
H(11A)	7201	-1263	4880	26(1)
H(11B)	7814	-1753	6161	26(1)
H(14A)	7206	-309	2749	26(1)
H(14B)	7740	-1674	3048	26(1)
H(15A)	5672	-965	5972	26(1)
H(15B)	6310	-2174	6041	26(1)
H(16A)	6053	-2982	7999	26(1)
H(16B)	5225	-2917	6968	26(1)
H(17A)	5115	-1905	8997	26(1)
H(17B)	4873	-827	7853	26(1)
H(18A)	6405	-887	9661	26(1)
H(18B)	5762	319	9560	26(1)
H(19A)	6804	1041	8545	26(1)
H(19B)	5972	988	7522	26(1)
H(27)	7912	-569	2081	50